

# FIGURE 1

## Amino acid sequence for full-length human wild type AIK [SEQ. ID No. 1]

(Residues 125-391 are underlined)

MDRSKENCIS	GPVKATAPVG	GPKRVLVTQQ	IPCQNPLPVN	SGQAQRVLCP	SNSSQRVPLQ	60
AQKLVSSHKP	VQNQKQKQLQ	ATSVPHPVSR	PLNNTQKSKQ	PLPSAPENNP	EEELASKQKN	120
EESKKRQWAL	EDFEIGRPLG	KGKFGNVYLA	REKQSKFILA	<u>LKVLFKAQLE</u>	KAGVEHQLR	180
<u>EVEIQSHLRH</u>	<u>PNILRLYGYF</u>	<u>HDATRVYLIL</u>	<u>EYAPLGTVYR</u>	<u>ELQKLSKFDE</u>	<u>QRTATYITEL</u>	240
<u>ANALSYCHSK</u>	<u>RVIHRDIKPE</u>	<u>NLLGGSAGEL</u>	<u>KIADFGWSVH</u>	<u>APSSRRTTLC</u>	<u>GTLDYLPPEM</u>	300
<u>IEGRMHDEKV</u>	<u>DLWSLGVLGY</u>	<u>EFLVGKPPFE</u>	<u>ANTYQETYKR</u>	<u>ISRVEFTFPD</u>	<u>FVTEGARDLI</u>	360
<u>SRLKHNPSQ</u>	<u>RPMLREVLEH</u>	<u>PWITANSSKP</u>	<u>SNCQNKESAS</u>	<u>KQS</u>		403

## Human cDNA sequence encoding residues 125-391 of AIK [SEQ. ID No. 2]

AAGAGGCAGT	GGGCTTTGGA	AGACTTTGAA	ATTGGTCGCC	CTCTGGGTAA	AGGAAAGTTT	60
GGTAATGTTT	ATTTGGCAAG	AGAAAAGCAA	AGCAAGTTTA	TTCTGGCTCT	TAAAGTGTTA	120
TTTAAAGCTC	AGCTGGAGAA	AGCCGGAGTG	GAGCATCAGC	TCAGAAAGAG	AGTAGAAATA	180
CAGTCCCACC	TTCGGCATCC	TAATATTCTT	AGACTGTATG	GTTATTTCCA	TGATGCTACC	240
AGAGTCTACC	TAATTCTGGA	ATATGCACCA	CTTGGAACAG	TTTATAGAGA	ACTTCAGAAA	300
CTTTCAAAGT	TTGATGAGCA	GAGAACTGCT	ACTTATATAA	CAGAATTGGC	AAATGCCCTG	360
TCTTACTGTC	ATTCTGAAGAG	AGTTATTTCAT	AGAGACATTA	AGCCAGAGAA	CTTACTTCTT	420
GGATCAGCTG	GAGAGCTTAA	AATTGCAGAT	TTTGGGTGGT	CAGTACATGC	TCCATCTTCC	480
AGGAGGACCA	CTCTCTGTGG	CACCCTGGAC	TACCTGCCCC	CTGAAATGAT	TGAAGGTCGG	540
ATGCATGATG	AGAAGGTGGA	TCTCTGGAGC	CTTGAGATTG	TTTGCTATGA	ATTTTTAGTT	600
GGGAAGCCTC	CTTTTGAGGC	AAACACATAC	CAAGAGACCT	ACAAAAGAAT	ATCACGGGTT	660
GAATTCACAT	TCCCTGACTT	TGTAACAGAG	GGAGCCAGGG	ACCTCATTTT	AAGACTGTTG	720
AAGCATAATC	CCAGCCAGAG	GCCAATGCTC	AGAGAAGTAC	TTGAACACCC	CTGGATCACA	780
GCAAATTCAT	CAAAACCATC	A				801

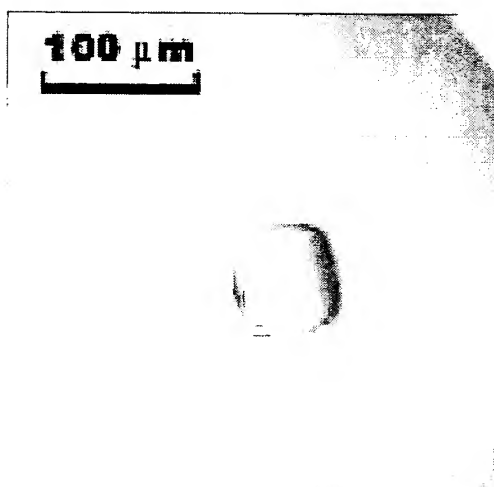
## Amino acid sequence for residues 125-391 of AIK with a cleavable

(rTev) N-terminal 6x-histidine tag [SEQ. ID No. 3]

(6x-histidine tag and cleavage site are underlined)

<u>MSYYHHHHHH</u>	<u>DYDIPTTENL</u>	<u>YFQGAMGSKR</u>	<u>QWALEDFEIG</u>	<u>RPLGKGKFGN</u>	<u>VYLAREKQSK</u>	60
<u>FILALKVLFK</u>	<u>AQLEKAGVEH</u>	<u>QLRREVEIQS</u>	<u>HLRHPNLR</u>	<u>YGYFHDATRV</u>	<u>YLILEYAPLG</u>	120
<u>TVYRELQKLS</u>	<u>KFDEQRTATY</u>	<u>ITELANALSY</u>	<u>CHSKRVIHRD</u>	<u>IKPENLLLGS</u>	<u>AGELKIADFG</u>	180
<u>WSVHAPSSRR</u>	<u>TTLCTGLDYL</u>	<u>PPEMIEGRMH</u>	<u>DEKVDLWSLG</u>	<u>VLCYEFLVGK</u>	<u>PPFEANTYQE</u>	240
<u>TYKRISRVEF</u>	<u>TFPDFVTEGA</u>	<u>RDLSRLLKH</u>	<u>NPSQRPMRE</u>	<u>VLEHPWITAN</u>	<u>SSKPS</u>	295

FIGURE 2



# FIGURE 3

## LEGEND

Column headings from left to right are (A)'Atom Number', (B)'Atom Type', (C)'Amino Acid', (D)'Chain Identifier', (E)'Amino Acid Number', (F)'X Coordinate', (G)'Y Coordinate', (H)'Z Coordinate', (I)'Occupancy' (OCC) and (J)'B factor'.

A	B	C	D	E	F	G	H	I	J
1	N	ALA	A	126	-1.225	18.275	58.949	1.00	62.30
2	CA	ALA	A	126	-0.160	18.687	59.906	1.00	61.70
3	CB	ALA	A	126	-0.351	20.162	60.315	1.00	62.19
4	C	ALA	A	126	-0.137	17.763	61.129	1.00	60.66
5	O	ALA	A	126	-0.940	17.908	62.044	1.00	61.53
6	N	ALA	A	127	0.784	16.805	61.123	1.00	59.08
7	CA	ALA	A	127	0.859	15.815	62.173	1.00	57.38
8	CB	ALA	A	127	1.255	14.482	61.599	1.00	57.77
9	C	ALA	A	127	1.878	16.247	63.205	1.00	56.23
10	O	ALA	A	127	3.075	16.075	63.000	1.00	56.65
11	N	TRP	A	128	1.401	16.816	64.301	1.00	53.28
12	CA	TRP	A	128	2.263	17.245	65.380	1.00	50.98
13	CB	TRP	A	128	1.566	18.369	66.133	1.00	51.50
14	CG	TRP	A	128	1.402	19.546	65.268	1.00	52.38
15	CD1	TRP	A	128	0.246	20.024	64.714	1.00	53.18
16	NE1	TRP	A	128	0.515	21.153	63.973	1.00	53.05
17	CE2	TRP	A	128	1.862	21.394	64.017	1.00	54.15
18	CD2	TRP	A	128	2.442	20.405	64.834	1.00	53.19
19	CE3	TRP	A	128	3.820	20.440	65.049	1.00	54.16
20	CZ3	TRP	A	128	4.554	21.416	64.458	1.00	53.73
21	CH2	TRP	A	128	3.949	22.391	63.660	1.00	54.15
22	CZ2	TRP	A	128	2.606	22.395	63.431	1.00	54.51
23	C	TRP	A	128	2.517	16.093	66.332	1.00	49.09
24	O	TRP	A	128	1.747	15.154	66.370	1.00	48.80
25	N	ALA	A	129	3.598	16.200	67.100	1.00	47.28
26	CA	ALA	A	129	3.992	15.236	68.114	1.00	46.51
27	CB	ALA	A	129	5.028	14.287	67.555	1.00	45.67
28	C	ALA	A	129	4.596	16.072	69.262	1.00	45.56
29	O	ALA	A	129	4.980	17.220	69.037	1.00	43.83
30	N	LEU	A	130	4.659	15.530	70.480	1.00	46.03
31	CA	LEU	A	130	5.155	16.302	71.628	1.00	46.26
32	CB	LEU	A	130	5.119	15.469	72.909	1.00	46.46
33	CG	LEU	A	130	4.612	16.028	74.261	1.00	49.12
34	CD1	LEU	A	130	5.469	15.546	75.419	1.00	47.91
35	CD2	LEU	A	130	4.470	17.523	74.311	1.00	46.43
36	C	LEU	A	130	6.570	16.796	71.348	1.00	46.06
37	O	LEU	A	130	6.933	17.927	71.722	1.00	45.86
38	N	GLU	A	131	7.349	15.967	70.657	1.00	44.57
39	CA	GLU	A	131	8.736	16.309	70.328	1.00	43.80
40	CB	GLU	A	131	9.506	15.118	69.669	1.00	45.34
41	CG	GLU	A	131	9.077	14.915	68.219	1.00	50.12
42	CD	GLU	A	131	9.560	13.599	67.616	1.00	59.64

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
43	OE1	GLU	A	131	8.836	13.078	66.726	1.00	64.32
44	OE2	GLU	A	131	10.648	13.084	67.993	1.00	63.67
45	C	GLU	A	131	8.937	17.577	69.485	1.00	41.74
46	O	GLU	A	131	10.041	18.101	69.415	1.00	41.77
47	N	ASP	A	132	7.881	18.078	68.841	1.00	39.05
48	CA	ASP	A	132	8.010	19.323	68.100	1.00	38.32
49	CB	ASP	A	132	6.935	19.466	67.028	1.00	39.96
50	CG	ASP	A	132	6.946	18.299	66.066	1.00	41.30
51	OD1	ASP	A	132	8.056	17.837	65.689	1.00	46.10
52	OD2	ASP	A	132	5.894	17.772	65.723	1.00	42.94
53	C	ASP	A	132	7.926	20.559	68.989	1.00	37.33
54	O	ASP	A	132	8.094	21.640	68.472	1.00	36.39
55	N	PHE	A	133	7.692	20.370	70.289	1.00	36.67
56	CA	PHE	A	133	7.485	21.498	71.213	1.00	37.49
57	CB	PHE	A	133	5.998	21.569	71.740	1.00	36.30
58	CG	PHE	A	133	4.958	21.474	70.656	1.00	38.62
59	CD1	PHE	A	133	4.504	22.602	69.999	1.00	38.46
60	CE1	PHE	A	133	3.564	22.499	68.993	1.00	41.24
61	CZ	PHE	A	133	3.108	21.250	68.611	1.00	39.81
62	CE2	PHE	A	133	3.564	20.125	69.246	1.00	38.63
63	CD2	PHE	A	133	4.495	20.235	70.252	1.00	39.61
64	C	PHE	A	133	8.475	21.593	72.399	1.00	38.04
65	O	PHE	A	133	8.934	20.578	72.922	1.00	37.77
66	N	GLU	A	134	8.825	22.817	72.801	1.00	37.74
67	CA	GLU	A	134	9.511	22.989	74.079	1.00	38.18
68	CB	GLU	A	134	10.583	24.031	73.989	1.00	38.70
69	CG	GLU	A	134	11.692	23.627	73.052	1.00	45.76
70	CD	GLU	A	134	12.863	24.551	73.142	1.00	52.60
71	OE1	GLU	A	134	14.009	24.040	72.996	1.00	57.17
72	OE2	GLU	A	134	12.635	25.768	73.380	1.00	57.77
73	C	GLU	A	134	8.424	23.456	74.979	1.00	37.78
74	O	GLU	A	134	7.697	24.400	74.647	1.00	37.67
75	N	ILE	A	135	8.295	22.825	76.123	1.00	35.90
76	CA	ILE	A	135	7.223	23.145	76.998	1.00	37.06
77	CB	ILE	A	135	6.657	21.878	77.499	1.00	37.79
78	CG1	ILE	A	135	5.960	21.157	76.334	1.00	41.64
79	CD1	ILE	A	135	4.794	20.341	76.792	1.00	48.55
80	CG2	ILE	A	135	5.700	22.126	78.593	1.00	37.59
81	C	ILE	A	135	7.682	24.058	78.152	1.00	36.78
82	O	ILE	A	135	8.778	23.906	78.672	1.00	34.54
83	N	GLY	A	136	6.819	24.998	78.533	1.00	37.69
84	CA	GLY	A	136	7.179	25.975	79.541	1.00	36.95
85	C	GLY	A	136	6.383	25.807	80.792	1.00	37.86
86	O	GLY	A	136	6.052	24.706	81.139	1.00	38.85
87	N	ARG	A	137	6.052	26.917	81.449	1.00	38.75
88	CA	ARG	A	137	5.311	26.886	82.699	1.00	39.01
89	CB	ARG	A	137	5.392	28.252	83.369	1.00	40.79
90	CG	ARG	A	137	4.941	29.390	82.494	1.00	39.62
91	CD	ARG	A	137	4.835	30.762	83.163	1.00	45.72
92	NE	ARG	A	137	3.554	30.754	83.754	1.00	48.61

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
93	CZ	ARG	A	137	2.501	31.519	83.484	1.00	42.31
94	NH1	ARG	A	137	2.481	32.576	82.674	1.00	39.40
95	NH2	ARG	A	137	1.423	31.205	84.148	1.00	40.08
96	C	ARG	A	137	3.841	26.591	82.437	1.00	38.31
97	O	ARG	A	137	3.319	26.884	81.363	1.00	35.25
98	N	PRO	A	138	3.186	26.035	83.432	1.00	38.59
99	CA	PRO	A	138	1.741	25.812	83.367	1.00	37.99
100	CB	PRO	A	138	1.416	25.119	84.688	1.00	38.79
101	CG	PRO	A	138	2.691	24.697	85.283	1.00	38.62
102	CD	PRO	A	138	3.782	25.569	84.712	1.00	40.69
103	C	PRO	A	138	1.059	27.163	83.333	1.00	37.95
104	O	PRO	A	138	1.369	28.068	84.123	1.00	36.30
105	N	LEU	A	139	0.165	27.313	82.368	1.00	37.66
106	CA	LEU	A	139	-0.617	28.512	82.249	1.00	35.85
107	CB	LEU	A	139	-1.012	28.701	80.804	1.00	34.42
108	CG	LEU	A	139	0.147	29.153	79.918	1.00	35.08
109	CD1	LEU	A	139	-0.222	29.021	78.419	1.00	33.54
110	CD2	LEU	A	139	0.576	30.644	80.230	1.00	35.10
111	C	LEU	A	139	-1.861	28.421	83.112	1.00	36.45
112	O	LEU	A	139	-2.410	29.451	83.532	1.00	35.77
113	N	GLY	A	140	-2.322	27.205	83.377	1.00	36.33
114	CA	GLY	A	140	-3.533	27.031	84.172	1.00	36.31
115	C	GLY	A	140	-3.900	25.579	84.428	1.00	37.85
116	O	GLY	A	140	-3.285	24.651	83.886	1.00	38.33
117	N	LYS	A	141	-4.872	25.372	85.301	1.00	38.89
118	CA	LYS	A	141	-5.255	24.016	85.681	1.00	40.43
119	CB	LYS	A	141	-5.479	23.905	87.204	1.00	41.81
120	CG	LYS	A	141	-4.305	23.314	88.006	1.00	47.61
121	CD	LYS	A	141	-4.581	23.141	89.534	1.00	54.52
122	CE	LYS	A	141	-4.243	24.411	90.322	1.00	58.25
123	NZ	LYS	A	141	-3.204	25.271	89.614	1.00	61.08
124	C	LYS	A	141	-6.575	23.809	84.999	1.00	39.72
125	O	LYS	A	141	-7.461	24.608	85.185	1.00	39.23
126	N	GLY	A	142	-6.677	22.773	84.167	1.00	39.64
127	CA	GLY	A	142	-7.934	22.410	83.523	1.00	40.24
128	C	GLY	A	142	-8.491	21.213	84.310	1.00	41.17
129	O	GLY	A	142	-7.897	20.741	85.294	1.00	41.10
130	N	LYS	A	143	-9.640	20.722	83.907	1.00	41.52
131	CA	LYS	A	143	-10.245	19.612	84.630	1.00	42.27
132	CB	LYS	A	143	-11.686	19.435	84.202	1.00	43.00
133	CG	LYS	A	143	-12.432	18.544	85.170	1.00	48.58
134	CD	LYS	A	143	-13.719	18.034	84.570	1.00	52.87
135	CE	LYS	A	143	-14.622	17.577	85.684	1.00	56.82
136	NZ	LYS	A	143	-14.896	16.117	85.592	1.00	61.41
137	C	LYS	A	143	-9.471	18.292	84.453	1.00	41.56
138	O	LYS	A	143	-9.248	17.572	85.412	1.00	40.75
139	N	PHE	A	144	-9.014	18.045	83.228	1.00	40.56
140	CA	PHE	A	144	-8.344	16.807	82.827	1.00	40.12
141	CB	PHE	A	144	-9.010	16.315	81.546	1.00	40.15
142	CG	PHE	A	144	-10.461	16.037	81.725	1.00	42.78
143	CD1	PHE	A	144	-10.877	14.867	82.383	1.00	45.37

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
144	CE1	PHE	A	144	-12.211	14.607	82.568	1.00	42.37
145	CZ	PHE	A	144	-13.160	15.517	82.120	1.00	44.22
146	CE2	PHE	A	144	-12.757	16.679	81.499	1.00	43.36
147	CD2	PHE	A	144	-11.420	16.948	81.315	1.00	39.89
148	C	PHE	A	144	-6.842	16.866	82.611	1.00	38.97
149	O	PHE	A	144	-6.253	15.909	82.150	1.00	36.84
150	N	GLY	A	145	-6.208	17.962	83.020	1.00	37.37
151	CA	GLY	A	145	-4.783	18.120	82.806	1.00	38.17
152	C	GLY	A	145	-4.486	19.606	82.814	1.00	37.75
153	O	GLY	A	145	-5.404	20.395	82.853	1.00	38.54
154	N	ASN	A	146	-3.230	19.999	82.753	1.00	38.01
155	CA	ASN	A	146	-2.930	21.412	82.804	1.00	37.94
156	CB	ASN	A	146	-1.619	21.626	83.563	1.00	38.27
157	CG	ASN	A	146	-1.718	21.186	85.022	1.00	43.37
158	OD1	ASN	A	146	-2.704	21.454	85.695	1.00	49.18
159	ND2	ASN	A	146	-0.698	20.506	85.499	1.00	48.99
160	C	ASN	A	146	-2.821	21.982	81.391	1.00	36.46
161	O	ASN	A	146	-2.732	21.209	80.411	1.00	35.01
162	N	VAL	A	147	-2.830	23.317	81.293	1.00	34.34
163	CA	VAL	A	147	-2.512	23.965	80.024	1.00	32.03
164	CB	VAL	A	147	-3.518	25.083	79.686	1.00	32.73
165	CG1	VAL	A	147	-3.098	25.767	78.335	1.00	31.49
166	CG2	VAL	A	147	-4.929	24.556	79.623	1.00	33.51
167	C	VAL	A	147	-1.081	24.524	80.153	1.00	32.07
168	O	VAL	A	147	-0.748	25.168	81.197	1.00	31.84
169	N	TYR	A	148	-0.227	24.312	79.148	1.00	29.65
170	CA	TYR	A	148	1.167	24.744	79.257	1.00	30.70
171	CB	TYR	A	148	2.135	23.546	79.082	1.00	30.68
172	CG	TYR	A	148	1.969	22.547	80.199	1.00	34.98
173	CD1	TYR	A	148	1.006	21.542	80.117	1.00	36.63
174	CE1	TYR	A	148	0.800	20.623	81.187	1.00	43.31
175	CZ	TYR	A	148	1.568	20.721	82.344	1.00	43.61
176	OH	TYR	A	148	1.362	19.826	83.394	1.00	45.34
177	CE2	TYR	A	148	2.513	21.730	82.456	1.00	43.40
178	CD2	TYR	A	148	2.719	22.648	81.356	1.00	40.12
179	C	TYR	A	148	1.532	25.740	78.197	1.00	30.72
180	O	TYR	A	148	1.079	25.648	77.054	1.00	30.29
181	N	LEU	A	149	2.386	26.675	78.554	1.00	30.08
182	CA	LEU	A	149	3.001	27.513	77.534	1.00	30.86
183	CB	LEU	A	149	3.880	28.526	78.247	1.00	32.09
184	CG	LEU	A	149	4.108	29.924	77.676	1.00	36.09
185	CD1	LEU	A	149	5.567	30.516	77.808	1.00	34.85
186	CD2	LEU	A	149	3.332	30.344	76.361	1.00	32.07
187	C	LEU	A	149	3.902	26.615	76.717	1.00	29.91
188	O	LEU	A	149	4.557	25.743	77.269	1.00	31.11
189	N	ALA	A	150	4.008	26.837	75.417	1.00	29.95
190	CA	ALA	A	150	4.879	25.986	74.645	1.00	29.87
191	CB	ALA	A	150	4.091	24.697	74.127	1.00	29.08
192	C	ALA	A	150	5.435	26.770	73.456	1.00	30.54
193	O	ALA	A	150	4.860	27.774	72.966	1.00	29.82
194	N	ARG	A	151	6.558	26.299	72.990	1.00	30.55

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
195	CA	ARG	A	151	7.164	26.847	71.809	1.00	32.81
196	CB	ARG	A	151	8.465	27.561	72.162	1.00	33.58
197	CG	ARG	A	151	8.864	28.606	71.141	1.00	34.41
198	CD	ARG	A	151	10.216	29.272	71.493	1.00	37.68
199	NE	ARG	A	151	11.314	28.358	71.774	1.00	41.98
200	CZ	ARG	A	151	12.579	28.754	71.840	1.00	45.91
201	NH1	ARG	A	151	12.855	30.033	71.642	1.00	45.17
202	NH2	ARG	A	151	13.554	27.891	72.109	1.00	48.67
203	C	ARG	A	151	7.393	25.735	70.792	1.00	33.58
204	O	ARG	A	151	7.806	24.623	71.151	1.00	36.75
205	N	GLU	A	152	6.998	26.037	69.557	1.00	35.31
206	CA	GLU	A	152	7.214	25.150	68.433	1.00	38.01
207	CB	GLU	A	152	6.339	25.554	67.232	1.00	38.19
208	CG	GLU	A	152	6.245	24.450	66.177	1.00	44.01
209	CD	GLU	A	152	7.475	24.363	65.241	1.00	48.90
210	OE1	GLU	A	152	7.735	25.334	64.489	1.00	52.00
211	OE2	GLU	A	152	8.192	23.320	65.250	1.00	51.05
212	C	GLU	A	152	8.677	25.296	68.065	1.00	37.84
213	O	GLU	A	152	9.161	26.382	67.791	1.00	38.28
214	N	LYS	A	153	9.392	24.200	68.043	1.00	39.21
215	CA	LYS	A	153	10.819	24.306	67.841	1.00	42.09
216	CB	LYS	A	153	11.481	22.967	68.153	1.00	42.63
217	CG	LYS	A	153	11.928	22.851	69.590	1.00	48.61
218	CD	LYS	A	153	11.539	21.510	70.175	1.00	55.42
219	CE	LYS	A	153	11.720	20.374	69.179	1.00	60.62
220	NZ	LYS	A	153	13.095	19.664	69.260	1.00	68.26
221	C	LYS	A	153	11.287	24.885	66.509	1.00	42.57
222	O	LYS	A	153	12.262	25.589	66.449	1.00	43.65
223	N	GLN	A	154	10.603	24.623	65.421	1.00	43.01
224	CA	GLN	A	154	11.158	25.126	64.163	1.00	44.19
225	CB	GLN	A	154	10.676	24.231	63.015	1.00	44.67
226	CG	GLN	A	154	11.442	22.952	63.045	1.00	53.28
227	CD	GLN	A	154	11.408	22.213	61.740	1.00	60.70
228	OE1	GLN	A	154	10.328	21.982	61.174	1.00	66.15
229	NE2	GLN	A	154	12.586	21.838	61.246	1.00	64.53
230	C	GLN	A	154	10.856	26.600	63.884	1.00	41.49
231	O	GLN	A	154	11.660	27.356	63.358	1.00	42.67
232	N	SER	A	155	9.675	27.022	64.254	1.00	38.39
233	CA	SER	A	155	9.313	28.371	63.946	1.00	35.68
234	CB	SER	A	155	7.840	28.364	63.594	1.00	34.74
235	OG	SER	A	155	7.196	27.875	64.746	1.00	34.70
236	C	SER	A	155	9.532	29.313	65.140	1.00	33.68
237	O	SER	A	155	9.505	30.517	64.946	1.00	33.85
238	N	LYS	A	156	9.672	28.739	66.331	1.00	32.82
239	CA	LYS	A	156	9.704	29.445	67.645	1.00	34.59
240	CB	LYS	A	156	10.858	30.467	67.753	1.00	34.66
241	CG	LYS	A	156	12.319	29.876	67.480	1.00	36.79
242	CD	LYS	A	156	13.429	30.907	67.970	1.00	44.57
243	CE	LYS	A	156	14.696	31.115	67.056	1.00	47.52
244	NZ	LYS	A	156	14.787	32.563	66.539	1.00	46.31
245	C	LYS	A	156	8.335	30.102	67.987	1.00	33.10

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
246	O	LYS	A	156	8.218	31.065	68.804	1.00	31.56
247	N	PHE	A	157	7.302	29.553	67.386	1.00	31.13
248	CA	PHE	A	157	5.948	30.020	67.646	1.00	31.45
249	CB	PHE	A	157	5.016	29.469	66.575	1.00	32.15
250	CG	PHE	A	157	3.713	30.177	66.469	1.00	34.87
251	CD1	PHE	A	157	3.527	31.155	65.492	1.00	38.48
252	CE1	PHE	A	157	2.274	31.786	65.329	1.00	40.08
253	CZ	PHE	A	157	1.209	31.427	66.143	1.00	37.15
254	CE2	PHE	A	157	1.368	30.425	67.104	1.00	34.69
255	CD2	PHE	A	157	2.644	29.795	67.253	1.00	36.13
256	C	PHE	A	157	5.466	29.641	69.057	1.00	29.29
257	O	PHE	A	157	5.395	28.469	69.412	1.00	29.48
258	N	ILE	A	158	5.022	30.656	69.813	1.00	29.61
259	CA	ILE	A	158	4.651	30.447	71.207	1.00	30.50
260	CB	ILE	A	158	4.899	31.717	72.032	1.00	31.00
261	CG1	ILE	A	158	6.366	31.797	72.339	1.00	36.27
262	CD1	ILE	A	158	6.687	30.925	73.512	1.00	37.94
263	CG2	ILE	A	158	4.419	31.510	73.466	1.00	32.23
264	C	ILE	A	158	3.209	30.163	71.230	1.00	29.07
265	O	ILE	A	158	2.473	30.911	70.644	1.00	30.88
266	N	LEU	A	159	2.745	29.157	71.935	1.00	28.37
267	CA	LEU	A	159	1.339	28.868	71.885	1.00	28.41
268	CB	LEU	A	159	1.085	27.936	70.692	1.00	28.97
269	CG	LEU	A	159	1.953	26.777	70.259	1.00	34.00
270	CD1	LEU	A	159	1.782	25.602	71.203	1.00	35.94
271	CD2	LEU	A	159	1.737	26.341	68.787	1.00	39.02
272	C	LEU	A	159	1.079	28.193	73.204	1.00	27.83
273	O	LEU	A	159	1.957	28.166	74.034	1.00	27.51
274	N	ALA	A	160	-0.120	27.685	73.409	1.00	29.15
275	CA	ALA	A	160	-0.450	27.016	74.661	1.00	30.37
276	CB	ALA	A	160	-1.651	27.684	75.323	1.00	28.84
277	C	ALA	A	160	-0.818	25.602	74.297	1.00	32.10
278	O	ALA	A	160	-1.472	25.371	73.269	1.00	31.99
279	N	LEU	A	161	-0.434	24.654	75.163	1.00	33.02
280	CA	LEU	A	161	-0.741	23.261	74.941	1.00	34.14
281	CB	LEU	A	161	0.577	22.495	74.913	1.00	34.88
282	CG	LEU	A	161	0.908	21.455	73.868	1.00	39.45
283	CD1	LEU	A	161	0.455	21.854	72.442	1.00	35.63
284	CD2	LEU	A	161	2.466	21.138	73.933	1.00	40.14
285	C	LEU	A	161	-1.648	22.780	76.036	1.00	33.03
286	O	LEU	A	161	-1.271	22.762	77.217	1.00	33.04
287	N	LYS	A	162	-2.885	22.456	75.657	1.00	31.43
288	CA	LYS	A	162	-3.856	21.979	76.610	1.00	32.34
289	CB	LYS	A	162	-5.251	22.451	76.196	1.00	32.99
290	CG	LYS	A	162	-6.391	21.951	77.087	1.00	29.62
291	CD	LYS	A	162	-7.595	22.831	76.855	1.00	29.33
292	CE	LYS	A	162	-8.841	22.204	77.533	1.00	27.32
293	NZ	LYS	A	162	-10.098	22.987	77.412	1.00	31.96
294	C	LYS	A	162	-3.772	20.441	76.654	1.00	33.11
295	O	LYS	A	162	-4.017	19.775	75.666	1.00	33.31
296	N	VAL	A	163	-3.364	19.907	77.790	1.00	35.02



**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
297	CA	VAL	A	163	-3.205	18.471	77.983	1.00	37.14
298	CB	VAL	A	163	-1.971	18.203	78.854	1.00	36.58
299	CG1	VAL	A	163	-1.720	16.660	79.039	1.00	37.74
300	CG2	VAL	A	163	-0.709	18.909	78.260	1.00	38.41
301	C	VAL	A	163	-4.445	17.854	78.653	1.00	37.59
302	O	VAL	A	163	-4.960	18.395	79.644	1.00	37.22
303	N	LEU	A	164	-4.977	16.767	78.073	1.00	39.14
304	CA	LEU	A	164	-6.104	16.048	78.686	1.00	39.01
305	CB	LEU	A	164	-7.427	16.202	77.930	1.00	39.22
306	CG	LEU	A	164	-7.961	17.622	77.781	1.00	38.09
307	CD1	LEU	A	164	-7.363	18.125	76.508	1.00	38.01
308	CD2	LEU	A	164	-9.453	17.647	77.711	1.00	37.35
309	C	LEU	A	164	-5.759	14.562	78.783	1.00	39.97
310	O	LEU	A	164	-5.369	13.952	77.798	1.00	38.76
311	N	PHE	A	165	-5.880	14.004	79.986	1.00	40.67
312	CA	PHE	A	165	-5.535	12.599	80.211	1.00	42.42
313	CB	PHE	A	165	-5.191	12.355	81.686	1.00	42.83
314	CG	PHE	A	165	-3.815	12.784	82.030	1.00	46.45
315	CD1	PHE	A	165	-3.573	14.040	82.560	1.00	47.62
316	CE1	PHE	A	165	-2.290	14.434	82.868	1.00	47.96
317	CZ	PHE	A	165	-1.227	13.574	82.628	1.00	50.56
318	CE2	PHE	A	165	-1.446	12.349	82.067	1.00	48.72
319	CD2	PHE	A	165	-2.740	11.951	81.775	1.00	48.08
320	C	PHE	A	165	-6.665	11.709	79.743	1.00	42.46
321	O	PHE	A	165	-7.788	11.832	80.199	1.00	40.57
322	N	LYS	A	166	-6.360	10.867	78.768	1.00	43.35
323	CA	LYS	A	166	-7.342	9.957	78.209	1.00	45.50
324	CB	LYS	A	166	-6.696	9.043	77.155	1.00	46.27
325	CG	LYS	A	166	-6.559	9.666	75.786	1.00	46.27
326	CD	LYS	A	166	-5.423	8.956	75.032	1.00	53.89
327	CE	LYS	A	166	-5.279	9.445	73.581	1.00	55.13
328	NZ	LYS	A	166	-5.709	8.444	72.569	1.00	59.86
329	C	LYS	A	166	-8.040	9.102	79.273	1.00	45.98
330	O	LYS	A	166	-9.230	8.981	79.250	1.00	46.56
331	N	ALA	A	167	-7.324	8.561	80.240	1.00	47.94
332	CA	ALA	A	167	-8.025	7.699	81.191	1.00	49.17
333	CB	ALA	A	167	-7.091	7.201	82.220	1.00	49.16
334	C	ALA	A	167	-9.168	8.457	81.848	1.00	49.92
335	O	ALA	A	167	-10.305	7.957	81.995	1.00	49.78
336	N	GLN	A	168	-8.859	9.696	82.218	1.00	49.84
337	CA	GLN	A	168	-9.787	10.502	82.960	1.00	49.29
338	CB	GLN	A	168	-9.058	11.694	83.591	1.00	50.22
339	CG	GLN	A	168	-8.451	11.419	84.993	1.00	54.78
340	CD	GLN	A	168	-7.028	10.830	84.965	1.00	62.45
341	OE1	GLN	A	168	-6.053	11.569	84.788	1.00	65.02
342	NE2	GLN	A	168	-6.908	9.511	85.190	1.00	64.80
343	C	GLN	A	168	-10.953	10.939	82.088	1.00	48.29
344	O	GLN	A	168	-12.085	10.976	82.553	1.00	47.87
345	N	LEU	A	169	-10.702	11.245	80.814	1.00	48.22
346	CA	LEU	A	169	-11.808	11.676	79.964	1.00	48.39
347	CB	LEU	A	169	-11.322	12.112	78.575	1.00	47.89

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
348	CG	LEU	A	169	-10.644	13.461	78.330	1.00	49.67
349	CD1	LEU	A	169	-10.181	13.552	76.882	1.00	48.91
350	CD2	LEU	A	169	-11.615	14.580	78.615	1.00	45.84
351	C	LEU	A	169	-12.819	10.538	79.785	1.00	47.86
352	O	LEU	A	169	-14.027	10.733	79.875	1.00	47.83
353	N	ALA	A	170	-12.316	9.368	79.451	1.00	48.31
354	CA	ALA	A	170	-13.220	8.238	79.195	1.00	48.55
355	CB	ALA	A	170	-12.468	7.070	78.581	1.00	49.34
356	C	ALA	A	170	-13.927	7.860	80.494	1.00	48.26
357	O	ALA	A	170	-15.118	7.692	80.501	1.00	49.17
358	N	ALA	A	171	-13.207	7.806	81.606	1.00	48.63
359	CA	ALA	A	171	-13.857	7.578	82.885	1.00	48.78
360	CB	ALA	A	171	-12.858	7.685	84.058	1.00	49.66
361	C	ALA	A	171	-14.996	8.561	83.082	1.00	48.71
362	O	ALA	A	171	-16.113	8.179	83.429	1.00	48.35
363	N	ALA	A	172	-14.723	9.841	82.844	1.00	48.29
364	CA	ALA	A	172	-15.740	10.846	83.012	1.00	47.44
365	CB	ALA	A	172	-15.093	12.246	83.064	1.00	48.07
366	C	ALA	A	172	-16.759	10.737	81.888	1.00	47.98
367	O	ALA	A	172	-17.893	11.232	81.984	1.00	48.40
368	N	GLY	A	173	-16.371	10.067	80.815	1.00	48.12
369	CA	GLY	A	173	-17.262	9.907	79.674	1.00	47.85
370	C	GLY	A	173	-17.733	11.166	78.995	1.00	47.73
371	O	GLY	A	173	-18.926	11.308	78.705	1.00	49.07
372	N	VAL	A	174	-16.790	12.075	78.736	1.00	46.88
373	CA	VAL	A	174	-17.030	13.322	78.021	1.00	45.99
374	CB	VAL	A	174	-16.674	14.572	78.873	1.00	45.74
375	CG1	VAL	A	174	-17.722	14.810	79.913	1.00	49.76
376	CG2	VAL	A	174	-15.330	14.425	79.472	1.00	46.00
377	C	VAL	A	174	-16.132	13.394	76.798	1.00	44.25
378	O	VAL	A	174	-15.792	14.483	76.300	1.00	43.32
379	N	ALA	A	175	-15.708	12.236	76.322	1.00	42.33
380	CA	ALA	A	175	-14.879	12.221	75.125	1.00	41.82
381	CB	ALA	A	175	-14.563	10.748	74.679	1.00	41.75
382	C	ALA	A	175	-15.577	13.026	74.008	1.00	40.98
383	O	ALA	A	175	-14.920	13.683	73.189	1.00	42.44
384	N	HIS	A	176	-16.899	13.030	74.009	1.00	40.16
385	CA	HIS	A	176	-17.657	13.751	72.980	1.00	41.39
386	CB	HIS	A	176	-19.146	13.385	73.068	1.00	41.58
387	CG	HIS	A	176	-19.803	13.903	74.318	1.00	45.86
388	ND1	HIS	A	176	-19.695	13.259	75.543	1.00	47.14
389	CE1	HIS	A	176	-20.355	13.949	76.460	1.00	47.79
390	NE2	HIS	A	176	-20.854	15.035	75.885	1.00	49.44
391	CD2	HIS	A	176	-20.532	15.023	74.545	1.00	46.34
392	C	HIS	A	176	-17.477	15.312	73.096	1.00	40.21
393	O	HIS	A	176	-17.529	16.043	72.107	1.00	38.56
394	N	GLN	A	177	-17.282	15.793	74.320	1.00	39.05
395	CA	GLN	A	177	-17.021	17.231	74.544	1.00	39.77
396	CB	GLN	A	177	-17.008	17.567	76.019	1.00	38.88
397	CG	GLN	A	177	-18.343	17.312	76.675	1.00	38.17
398	CD	GLN	A	177	-18.467	17.978	78.032	1.00	36.45

# FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
399	OE1	GLN	A	177	-19.540	18.436	78.382	1.00	43.55
400	NE2	GLN	A	177	-17.393	17.992	78.801	1.00	32.42
401	C	GLN	A	177	-15.672	17.586	73.966	1.00	39.55
402	O	GLN	A	177	-15.519	18.636	73.379	1.00	40.58
403	N	LEU	A	178	-14.691	16.722	74.144	1.00	38.53
404	CA	LEU	A	178	-13.396	17.016	73.556	1.00	38.40
405	CB	LEU	A	178	-12.332	16.028	73.974	1.00	37.56
406	CG	LEU	A	178	-10.937	16.463	73.548	1.00	39.19
407	CD1	LEU	A	178	-10.647	17.912	74.074	1.00	42.88
408	CD2	LEU	A	178	-9.892	15.543	74.112	1.00	42.48
409	C	LEU	A	178	-13.537	17.041	72.039	1.00	38.85
410	O	LEU	A	178	-12.977	17.902	71.384	1.00	38.48
411	N	ARG	A	179	-14.362	16.156	71.478	1.00	38.80
412	CA	ARG	A	179	-14.528	16.156	70.027	1.00	38.95
413	CB	ARG	A	179	-15.552	15.134	69.583	1.00	41.23
414	CG	ARG	A	179	-15.211	14.622	68.199	1.00	45.48
415	CD	ARG	A	179	-15.384	13.090	68.099	1.00	56.58
416	NE	ARG	A	179	-16.441	12.637	69.012	1.00	57.68
417	CZ	ARG	A	179	-16.275	11.730	69.973	1.00	57.26
418	NH1	ARG	A	179	-17.291	11.381	70.749	1.00	53.81
419	NH2	ARG	A	179	-15.093	11.162	70.159	1.00	59.58
420	C	ARG	A	179	-15.092	17.456	69.558	1.00	38.62
421	O	ARG	A	179	-14.762	17.995	68.508	1.00	38.21
422	N	ARG	A	180	-16.042	17.943	70.318	1.00	39.35
423	CA	ARG	A	180	-16.739	19.126	69.851	1.00	41.02
424	CB	ARG	A	180	-18.096	19.338	70.575	1.00	41.10
425	CG	ARG	A	180	-19.359	19.248	69.686	1.00	48.65
426	CD	ARG	A	180	-20.364	18.182	70.125	1.00	56.75
427	NE	ARG	A	180	-20.662	18.254	71.551	1.00	60.82
428	CZ	ARG	A	180	-21.716	17.672	72.127	1.00	64.30
429	NH1	ARG	A	180	-21.941	17.819	73.430	1.00	64.17
430	NH2	ARG	A	180	-22.566	16.958	71.400	1.00	65.87
431	C	ARG	A	180	-15.888	20.374	69.923	1.00	39.65
432	O	ARG	A	180	-15.924	21.204	69.026	1.00	38.25
433	N	GLU	A	181	-15.136	20.501	71.003	1.00	39.01
434	CA	GLU	A	181	-14.302	21.665	71.254	1.00	38.98
435	CB	GLU	A	181	-13.453	21.368	72.514	1.00	39.58
436	CG	GLU	A	181	-12.421	22.429	72.937	1.00	41.25
437	CD	GLU	A	181	-11.926	22.254	74.396	1.00	44.88
438	OE1	GLU	A	181	-10.944	22.921	74.792	1.00	48.21
439	OE2	GLU	A	181	-12.528	21.477	75.192	1.00	45.90
440	C	GLU	A	181	-13.361	21.802	70.074	1.00	38.90
441	O	GLU	A	181	-13.111	22.894	69.576	1.00	38.31
442	N	VAL	A	182	-12.803	20.667	69.651	1.00	38.34
443	CA	VAL	A	182	-11.850	20.639	68.537	1.00	38.73
444	CB	VAL	A	182	-11.090	19.274	68.390	1.00	40.09
445	CG1	VAL	A	182	-10.416	19.128	66.980	1.00	40.39
446	CG2	VAL	A	182	-10.051	19.079	69.506	1.00	38.26
447	C	VAL	A	182	-12.541	20.959	67.237	1.00	38.65
448	O	VAL	A	182	-12.119	21.839	66.516	1.00	39.07
449	N	ALA	A	183	-13.656	20.285	66.957	1.00	39.36

# FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
450	CA	ALA	A	183	-14.312	20.503	65.679	1.00	40.14
451	CB	ALA	A	183	-15.334	19.370	65.405	1.00	41.08
452	C	ALA	A	183	-14.965	21.870	65.636	1.00	40.80
453	O	ALA	A	183	-14.972	22.545	64.609	1.00	41.84
454	N	ILE	A	184	-15.524	22.312	66.748	1.00	38.99
455	CA	ILE	A	184	-16.157	23.595	66.678	1.00	39.48
456	CB	ILE	A	184	-17.210	23.754	67.766	1.00	38.90
457	CG1	ILE	A	184	-18.387	22.819	67.472	1.00	42.19
458	CD1	ILE	A	184	-19.459	22.799	68.584	1.00	40.68
459	CG2	ILE	A	184	-17.715	25.164	67.777	1.00	40.73
460	C	ILE	A	184	-15.124	24.703	66.747	1.00	39.32
461	O	ILE	A	184	-15.148	25.635	65.929	1.00	38.88
462	N	GLN	A	185	-14.209	24.612	67.723	1.00	38.82
463	CA	GLN	A	185	-13.281	25.717	67.911	1.00	38.20
464	CB	GLN	A	185	-12.446	25.531	69.185	1.00	38.61
465	CG	GLN	A	185	-12.426	26.806	70.015	1.00	36.79
466	CD	GLN	A	185	-11.623	26.663	71.277	1.00	38.97
467	OE1	GLN	A	185	-10.817	27.519	71.599	1.00	35.32
468	NE2	GLN	A	185	-11.869	25.627	71.997	1.00	32.38
469	C	GLN	A	185	-12.337	25.905	66.754	1.00	38.81
470	O	GLN	A	185	-11.936	27.027	66.479	1.00	37.38
471	N	SER	A	186	-11.946	24.823	66.083	1.00	39.57
472	CA	SER	A	186	-10.957	25.005	65.007	1.00	41.86
473	CB	SER	A	186	-10.302	23.684	64.569	1.00	41.93
474	OG	SER	A	186	-11.289	22.671	64.412	1.00	42.48
475	C	SER	A	186	-11.509	25.748	63.798	1.00	42.50
476	O	SER	A	186	-10.761	26.297	63.017	1.00	43.08
477	N	HIS	A	187	-12.817	25.781	63.656	1.00	43.53
478	CA	HIS	A	187	-13.397	26.411	62.471	1.00	45.61
479	CB	HIS	A	187	-14.585	25.580	61.955	1.00	46.41
480	CG	HIS	A	187	-14.173	24.264	61.396	1.00	52.65
481	ND1	HIS	A	187	-14.352	23.934	60.072	1.00	58.39
482	CE1	HIS	A	187	-13.863	22.725	59.855	1.00	58.68
483	NE2	HIS	A	187	-13.354	22.269	60.986	1.00	59.03
484	CD2	HIS	A	187	-13.527	23.215	61.965	1.00	56.31
485	C	HIS	A	187	-13.815	27.843	62.684	1.00	44.76
486	O	HIS	A	187	-13.962	28.608	61.725	1.00	44.78
487	N	LEU	A	188	-13.984	28.229	63.945	1.00	44.38
488	CA	LEU	A	188	-14.351	29.612	64.257	1.00	43.43
489	CB	LEU	A	188	-14.767	29.748	65.747	1.00	43.01
490	CG	LEU	A	188	-15.964	28.891	66.146	1.00	43.56
491	CD1	LEU	A	188	-16.328	29.051	67.640	1.00	41.71
492	CD2	LEU	A	188	-17.109	29.282	65.302	1.00	41.54
493	C	LEU	A	188	-13.143	30.477	64.001	1.00	42.37
494	O	LEU	A	188	-12.036	30.079	64.321	1.00	43.11
495	N	ARG	A	189	-13.365	31.677	63.478	1.00	42.12
496	CA	ARG	A	189	-12.293	32.644	63.200	1.00	42.01
497	CB	ARG	A	189	-11.962	32.682	61.695	1.00	42.31
498	CG	ARG	A	189	-11.239	31.477	61.229	1.00	44.33
499	CD	ARG	A	189	-9.871	31.267	61.898	1.00	46.81
500	NE	ARG	A	189	-9.128	30.280	61.109	1.00	54.20

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
501	CZ	ARG	A	189	-9.335	28.979	61.187	1.00	56.68
502	NH1	ARG	A	189	-8.643	28.153	60.419	1.00	58.82
503	NH2	ARG	A	189	-10.230	28.496	62.049	1.00	57.84
504	C	ARG	A	189	-12.809	34.010	63.580	1.00	41.15
505	O	ARG	A	189	-13.554	34.620	62.819	1.00	41.64
506	N	HIS	A	190	-12.402	34.506	64.739	1.00	40.04
507	CA	HIS	A	190	-12.901	35.775	65.194	1.00	38.65
508	CB	HIS	A	190	-14.316	35.605	65.760	1.00	38.81
509	CG	HIS	A	190	-14.925	36.886	66.202	1.00	39.63
510	ND1	HIS	A	190	-15.866	37.557	65.454	1.00	40.19
511	CE1	HIS	A	190	-16.189	38.680	66.071	1.00	37.93
512	NE2	HIS	A	190	-15.486	38.762	67.184	1.00	36.58
513	CD2	HIS	A	190	-14.671	37.664	67.284	1.00	33.70
514	C	HIS	A	190	-11.906	36.363	66.185	1.00	37.98
515	O	HIS	A	190	-11.329	35.649	66.986	1.00	38.30
516	N	PRO	A	191	-11.640	37.657	66.113	1.00	38.45
517	CA	PRO	A	191	-10.581	38.239	66.953	1.00	36.82
518	CB	PRO	A	191	-10.615	39.701	66.553	1.00	37.97
519	CG	PRO	A	191	-12.033	39.881	66.066	1.00	38.87
520	CD	PRO	A	191	-12.253	38.668	65.234	1.00	38.97
521	C	PRO	A	191	-10.903	38.055	68.457	1.00	35.66
522	O	PRO	A	191	-9.992	38.127	69.276	1.00	34.96
523	N	ASN	A	192	-12.158	37.814	68.804	1.00	34.30
524	CA	ASN	A	192	-12.523	37.581	70.217	1.00	33.52
525	CB	ASN	A	192	-13.612	38.556	70.663	1.00	32.97
526	CG	ASN	A	192	-13.207	40.027	70.497	1.00	35.71
527	OD1	ASN	A	192	-12.286	40.503	71.178	1.00	35.61
528	ND2	ASN	A	192	-13.823	40.714	69.556	1.00	31.27
529	C	ASN	A	192	-12.871	36.123	70.646	1.00	32.20
530	O	ASN	A	192	-13.603	35.887	71.624	1.00	31.19
531	N	ILE	A	193	-12.368	35.159	69.890	1.00	30.72
532	CA	ILE	A	193	-12.535	33.743	70.202	1.00	31.30
533	CB	ILE	A	193	-13.428	33.071	69.151	1.00	31.25
534	CG1	ILE	A	193	-14.862	33.600	69.252	1.00	32.94
535	CD1	ILE	A	193	-15.777	33.149	68.134	1.00	36.50
536	CG2	ILE	A	193	-13.371	31.550	69.293	1.00	29.33
537	C	ILE	A	193	-11.166	33.124	70.102	1.00	30.85
538	O	ILE	A	193	-10.472	33.376	69.121	1.00	31.20
539	N	LEU	A	194	-10.764	32.311	71.085	1.00	29.48
540	CA	LEU	A	194	-9.497	31.652	71.065	1.00	30.26
541	CB	LEU	A	194	-9.165	31.043	72.422	1.00	28.89
542	CG	LEU	A	194	-7.685	30.760	72.565	1.00	31.38
543	CD1	LEU	A	194	-6.957	32.083	72.928	1.00	27.79
544	CD2	LEU	A	194	-7.565	29.741	73.655	1.00	30.09
545	C	LEU	A	194	-9.417	30.580	69.984	1.00	30.59
546	O	LEU	A	194	-10.224	29.651	69.930	1.00	31.64
547	N	ARG	A	195	-8.411	30.745	69.139	1.00	31.20
548	CA	ARG	A	195	-8.121	29.904	68.003	1.00	32.25
549	CB	ARG	A	195	-7.026	30.648	67.258	1.00	33.95
550	CG	ARG	A	195	-6.742	30.234	65.886	1.00	42.54
551	CD	ARG	A	195	-7.805	30.522	64.863	1.00	46.96

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
552	NE	ARG	A	195	-7.275	29.900	63.663	1.00	52.66
553	CZ	ARG	A	195	-6.358	30.480	62.912	1.00	56.14
554	NH1	ARG	A	195	-5.941	31.694	63.224	1.00	56.04
555	NH2	ARG	A	195	-5.861	29.867	61.844	1.00	60.45
556	C	ARG	A	195	-7.580	28.611	68.529	1.00	30.98
557	O	ARG	A	195	-6.771	28.614	69.450	1.00	28.95
558	N	LEU	A	196	-8.015	27.509	67.984	1.00	31.25
559	CA	LEU	A	196	-7.440	26.226	68.277	1.00	31.50
560	CB	LEU	A	196	-8.517	25.265	68.720	1.00	32.30
561	CG	LEU	A	196	-8.057	23.870	69.131	1.00	33.64
562	CD1	LEU	A	196	-9.058	23.370	70.151	1.00	36.24
563	CD2	LEU	A	196	-8.117	23.052	67.904	1.00	34.95
564	C	LEU	A	196	-6.795	25.867	66.932	1.00	35.11
565	O	LEU	A	196	-7.445	25.957	65.875	1.00	34.69
566	N	TYR	A	197	-5.509	25.518	66.972	1.00	36.02
567	CA	TYR	A	197	-4.765	25.276	65.763	1.00	37.91
568	CB	TYR	A	197	-3.331	25.747	65.950	1.00	39.49
569	CG	TYR	A	197	-3.243	27.233	66.128	1.00	40.35
570	CD1	TYR	A	197	-2.704	27.782	67.278	1.00	43.33
571	CE1	TYR	A	197	-2.619	29.122	67.439	1.00	43.54
572	CZ	TYR	A	197	-3.072	29.953	66.451	1.00	44.37
573	OH	TYR	A	197	-2.949	31.310	66.604	1.00	48.37
574	CE2	TYR	A	197	-3.603	29.455	65.296	1.00	45.10
575	CD2	TYR	A	197	-3.697	28.087	65.139	1.00	44.72
576	C	TYR	A	197	-4.762	23.826	65.380	1.00	38.77
577	O	TYR	A	197	-4.536	23.490	64.216	1.00	39.64
578	N	GLY	A	198	-4.976	22.955	66.351	1.00	37.60
579	CA	GLY	A	198	-5.013	21.553	66.019	1.00	38.52
580	C	GLY	A	198	-4.785	20.771	67.265	1.00	38.86
581	O	GLY	A	198	-4.900	21.311	68.409	1.00	36.64
582	N	TYR	A	199	-4.428	19.511	67.066	1.00	38.68
583	CA	TYR	A	199	-4.334	18.597	68.185	1.00	40.56
584	CB	TYR	A	199	-5.731	18.163	68.637	1.00	39.96
585	CG	TYR	A	199	-6.334	17.067	67.753	1.00	44.40
586	CD1	TYR	A	199	-7.074	17.385	66.618	1.00	44.98
587	CE1	TYR	A	199	-7.626	16.382	65.807	1.00	48.78
588	CZ	TYR	A	199	-7.420	15.058	66.132	1.00	50.76
589	OH	TYR	A	199	-7.947	14.040	65.357	1.00	58.47
590	CE2	TYR	A	199	-6.697	14.722	67.244	1.00	51.67
591	CD2	TYR	A	199	-6.160	15.736	68.060	1.00	46.05
592	C	TYR	A	199	-3.517	17.369	67.877	1.00	40.55
593	O	TYR	A	199	-3.291	17.055	66.728	1.00	40.45
594	N	PHE	A	200	-3.066	16.670	68.911	1.00	40.86
595	CA	PHE	A	200	-2.416	15.411	68.656	1.00	42.07
596	CB	PHE	A	200	-0.963	15.636	68.198	1.00	41.03
597	CG	PHE	A	200	-0.122	16.422	69.173	1.00	44.63
598	CD1	PHE	A	200	0.713	15.760	70.035	1.00	42.87
599	CE1	PHE	A	200	1.515	16.436	70.934	1.00	44.73
600	CZ	PHE	A	200	1.477	17.801	71.010	1.00	43.50
601	CE2	PHE	A	200	0.655	18.492	70.162	1.00	43.78
602	CD2	PHE	A	200	-0.191	17.817	69.254	1.00	43.04

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
603	C	PHE	A	200	-2.610	14.522	69.888	1.00	42.82
604	O	PHE	A	200	-3.188	14.961	70.897	1.00	39.88
605	N	HIS	A	201	-2.268	13.251	69.770	1.00	44.66
606	CA	HIS	A	201	-2.394	12.350	70.911	1.00	48.80
607	CB	HIS	A	201	-3.807	11.739	70.991	1.00	49.16
608	CG	HIS	A	201	-4.132	10.793	69.870	1.00	53.25
609	ND1	HIS	A	201	-3.940	9.429	69.956	1.00	57.68
610	CE1	HIS	A	201	-4.339	8.855	68.832	1.00	58.86
611	NE2	HIS	A	201	-4.794	9.797	68.024	1.00	58.83
612	CD2	HIS	A	201	-4.676	11.018	68.650	1.00	57.09
613	C	HIS	A	201	-1.323	11.281	70.980	1.00	49.89
614	O	HIS	A	201	-0.807	10.810	69.960	1.00	50.59
615	N	ASP	A	202	-0.983	10.943	72.219	1.00	52.70
616	CA	ASP	A	202	-0.084	9.828	72.492	1.00	53.99
617	CB	ASP	A	202	1.241	10.287	73.079	1.00	54.12
618	CG	ASP	A	202	1.098	10.887	74.444	1.00	55.69
619	OD1	ASP	A	202	0.064	10.619	75.099	1.00	54.93
620	OD2	ASP	A	202	2.000	11.609	74.943	1.00	54.23
621	C	ASP	A	202	-0.819	8.790	73.330	1.00	54.16
622	O	ASP	A	202	-2.064	8.730	73.308	1.00	54.26
623	N	ALA	A	203	-0.084	7.976	74.067	1.00	54.51
624	CA	ALA	A	203	-0.738	6.843	74.732	1.00	54.56
625	CB	ALA	A	203	0.314	5.869	75.285	1.00	54.78
626	C	ALA	A	203	-1.716	7.242	75.824	1.00	54.14
627	O	ALA	A	203	-2.869	6.753	75.887	1.00	54.14
628	N	THR	A	204	-1.254	8.141	76.681	1.00	52.74
629	CA	THR	A	204	-2.040	8.535	77.833	1.00	51.77
630	CB	THR	A	204	-1.114	8.467	79.073	1.00	52.77
631	OG1	THR	A	204	-1.821	8.827	80.286	1.00	56.55
632	CG2	THR	A	204	-0.003	9.483	78.940	1.00	51.61
633	C	THR	A	204	-2.689	9.929	77.704	1.00	50.02
634	O	THR	A	204	-3.546	10.290	78.496	1.00	48.39
635	N	ARG	A	205	-2.312	10.702	76.693	1.00	48.75
636	CA	ARG	A	205	-2.797	12.093	76.643	1.00	47.39
637	CB	ARG	A	205	-1.740	13.047	77.192	1.00	47.22
638	CG	ARG	A	205	-1.295	12.746	78.573	1.00	50.14
639	CD	ARG	A	205	0.224	12.732	78.698	1.00	59.09
640	NE	ARG	A	205	0.805	13.946	79.262	1.00	65.81
641	CZ	ARG	A	205	2.118	14.116	79.455	1.00	71.17
642	NH1	ARG	A	205	2.587	15.256	79.974	1.00	73.74
643	NH2	ARG	A	205	2.968	13.142	79.123	1.00	72.85
644	C	ARG	A	205	-3.228	12.598	75.293	1.00	44.76
645	O	ARG	A	205	-2.831	12.070	74.258	1.00	44.49
646	N	VAL	A	206	-4.119	13.582	75.354	1.00	42.03
647	CA	VAL	A	206	-4.578	14.339	74.206	1.00	40.02
648	CB	VAL	A	206	-6.136	14.273	74.061	1.00	40.51
649	CG1	VAL	A	206	-6.638	15.182	72.954	1.00	41.85
650	CG2	VAL	A	206	-6.580	12.851	73.737	1.00	41.32
651	C	VAL	A	206	-4.039	15.785	74.414	1.00	38.80
652	O	VAL	A	206	-3.996	16.298	75.539	1.00	38.31
653	N	TYR	A	207	-3.593	16.409	73.341	1.00	37.44
654	CA	TYR	A	207	-2.976	17.737	73.430	1.00	38.03

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
655	CB	TYR	A	207	-1.549	17.670	72.968	1.00	36.40
656	CG	TYR	A	207	-0.688	16.778	73.766	1.00	39.00
657	CD1	TYR	A	207	-0.010	17.249	74.881	1.00	39.70
658	CE1	TYR	A	207	0.818	16.417	75.590	1.00	44.38
659	CZ	TYR	A	207	0.948	15.092	75.187	1.00	45.91
660	OH	TYR	A	207	1.734	14.246	75.900	1.00	50.45
661	CE2	TYR	A	207	0.290	14.609	74.090	1.00	43.62
662	CD2	TYR	A	207	-0.539	15.439	73.398	1.00	40.40
663	C	TYR	A	207	-3.595	18.728	72.511	1.00	37.21
664	O	TYR	A	207	-3.384	18.643	71.286	1.00	39.25
665	N	LEU	A	208	-4.323	19.685	73.049	1.00	35.21
666	CA	LEU	A	208	-4.858	20.693	72.172	1.00	32.76
667	CB	LEU	A	208	-6.177	21.235	72.710	1.00	32.84
668	CG	LEU	A	208	-7.403	20.429	72.312	1.00	36.54
669	CD1	LEU	A	208	-7.148	18.880	72.249	1.00	39.94
670	CD2	LEU	A	208	-8.584	20.792	73.169	1.00	34.97
671	C	LEU	A	208	-3.851	21.827	71.975	1.00	31.94
672	O	LEU	A	208	-3.292	22.378	72.960	1.00	31.89
673	N	ILE	A	209	-3.605	22.175	70.710	1.00	27.64
674	CA	ILE	A	209	-2.719	23.286	70.374	1.00	29.03
675	CB	ILE	A	209	-2.034	23.047	69.043	1.00	29.46
676	CG1	ILE	A	209	-1.424	21.632	68.983	1.00	33.03
677	CD1	ILE	A	209	-0.629	21.353	67.616	1.00	36.54
678	CG2	ILE	A	209	-0.996	24.092	68.833	1.00	27.57
679	C	ILE	A	209	-3.518	24.572	70.249	1.00	29.27
680	O	ILE	A	209	-4.206	24.763	69.258	1.00	30.08
681	N	LEU	A	210	-3.372	25.462	71.226	1.00	27.89
682	CA	LEU	A	210	-4.143	26.671	71.304	1.00	28.36
683	CB	LEU	A	210	-4.768	26.757	72.729	1.00	26.97
684	CG	LEU	A	210	-5.603	25.569	73.209	1.00	31.79
685	CD1	LEU	A	210	-6.165	25.926	74.613	1.00	31.27
686	CD2	LEU	A	210	-6.798	25.282	72.204	1.00	34.08
687	C	LEU	A	210	-3.346	27.967	71.066	1.00	26.61
688	O	LEU	A	210	-2.177	28.060	71.382	1.00	27.93
689	N	GLU	A	211	-3.994	28.972	70.520	1.00	29.15
690	CA	GLU	A	211	-3.501	30.350	70.621	1.00	29.81
691	CB	GLU	A	211	-4.498	31.350	70.047	1.00	31.22
692	CG	GLU	A	211	-3.984	32.779	70.020	1.00	35.70
693	CD	GLU	A	211	-5.147	33.799	70.050	1.00	39.08
694	OE1	GLU	A	211	-4.932	34.950	70.489	1.00	43.39
695	OE2	GLU	A	211	-6.288	33.455	69.653	1.00	38.36
696	C	GLU	A	211	-3.161	30.663	72.128	1.00	29.58
697	O	GLU	A	211	-3.948	30.404	73.014	1.00	28.54
698	N	TYR	A	212	-1.957	31.153	72.381	1.00	28.23
699	CA	TYR	A	212	-1.550	31.606	73.725	1.00	28.20
700	CB	TYR	A	212	-0.028	31.697	73.739	1.00	28.08
701	CG	TYR	A	212	0.592	32.494	74.874	1.00	29.44
702	CD1	TYR	A	212	1.521	33.489	74.601	1.00	30.49
703	CE1	TYR	A	212	2.131	34.197	75.639	1.00	36.30
704	CZ	TYR	A	212	1.773	33.945	76.903	1.00	33.49
705	OH	TYR	A	212	2.383	34.655	77.887	1.00	37.20



**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
706	CE2	TYR	A	212	0.802	32.977	77.225	1.00	33.16
707	CD2	TYR	A	212	0.234	32.258	76.188	1.00	28.40
708	C	TYR	A	212	-2.183	33.022	74.034	1.00	28.48
709	O	TYR	A	212	-2.089	33.924	73.211	1.00	27.53
710	N	ALA	A	213	-2.836	33.156	75.205	1.00	28.23
711	CA	ALA	A	213	-3.431	34.424	75.650	1.00	30.33
712	CB	ALA	A	213	-4.884	34.284	76.103	1.00	28.94
713	C	ALA	A	213	-2.550	34.953	76.780	1.00	30.02
714	O	ALA	A	213	-2.634	34.540	77.872	1.00	31.02
715	N	PRO	A	214	-1.720	35.904	76.442	1.00	31.54
716	CA	PRO	A	214	-0.632	36.365	77.313	1.00	32.57
717	CB	PRO	A	214	0.219	37.264	76.395	1.00	32.48
718	CG	PRO	A	214	-0.495	37.305	75.047	1.00	35.80
719	CD	PRO	A	214	-1.853	36.639	75.171	1.00	30.79
720	C	PRO	A	214	-1.070	37.096	78.596	1.00	34.06
721	O	PRO	A	214	-0.408	36.972	79.644	1.00	35.53
722	N	LEU	A	215	-2.187	37.789	78.548	1.00	33.98
723	CA	LEU	A	215	-2.641	38.503	79.718	1.00	36.04
724	CB	LEU	A	215	-3.341	39.786	79.296	1.00	34.70
725	CG	LEU	A	215	-2.394	41.003	79.195	1.00	36.83
726	CD1	LEU	A	215	-1.157	40.725	78.377	1.00	35.83
727	CD2	LEU	A	215	-3.180	42.190	78.627	1.00	35.88
728	C	LEU	A	215	-3.521	37.689	80.677	1.00	35.81
729	O	LEU	A	215	-4.121	38.247	81.571	1.00	35.82
730	N	GLY	A	216	-3.603	36.381	80.470	1.00	35.32
731	CA	GLY	A	216	-4.326	35.503	81.372	1.00	34.32
732	C	GLY	A	216	-5.848	35.530	81.287	1.00	32.64
733	O	GLY	A	216	-6.426	35.895	80.257	1.00	32.48
734	N	THR	A	217	-6.500	35.138	82.367	1.00	31.56
735	CA	THR	A	217	-7.962	35.119	82.396	1.00	31.29
736	CB	THR	A	217	-8.511	33.951	83.212	1.00	32.13
737	OG1	THR	A	217	-8.082	34.088	84.587	1.00	30.67
738	CG2	THR	A	217	-7.974	32.629	82.730	1.00	31.12
739	C	THR	A	217	-8.613	36.355	83.020	1.00	31.68
740	O	THR	A	217	-8.041	37.069	83.856	1.00	28.84
741	N	VAL	A	218	-9.881	36.498	82.686	1.00	30.86
742	CA	VAL	A	218	-10.694	37.528	83.283	1.00	32.14
743	CB	VAL	A	218	-11.953	37.675	82.526	1.00	33.13
744	CG1	VAL	A	218	-12.978	38.466	83.328	1.00	35.75
745	CG2	VAL	A	218	-11.616	38.289	81.172	1.00	31.98
746	C	VAL	A	218	-10.920	37.150	84.768	1.00	32.06
747	O	VAL	A	218	-11.039	38.023	85.642	1.00	32.00
748	N	TYR	A	219	-10.958	35.849	85.032	1.00	32.11
749	CA	TYR	A	219	-11.062	35.374	86.402	1.00	33.66
750	CB	TYR	A	219	-11.049	33.838	86.406	1.00	33.98
751	CG	TYR	A	219	-11.116	33.234	87.785	1.00	35.91
752	CD1	TYR	A	219	-12.335	32.895	88.354	1.00	38.53
753	CE1	TYR	A	219	-12.412	32.339	89.620	1.00	46.18
754	CZ	TYR	A	219	-11.236	32.109	90.335	1.00	47.58
755	OH	TYR	A	219	-11.326	31.532	91.592	1.00	53.35
756	CE2	TYR	A	219	-10.001	32.451	89.785	1.00	42.92

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
757	CD2	TYR	A	219	-9.954	32.999	88.517	1.00	37.24
758	C	TYR	A	219	-9.883	35.936	87.269	1.00	33.62
759	O	TYR	A	219	-10.105	36.423	88.379	1.00	33.27
760	N	ARG	A	220	-8.703	35.924	86.725	1.00	34.37
761	CA	ARG	A	220	-7.506	36.322	87.508	1.00	36.06
762	CB	ARG	A	220	-6.243	35.827	86.810	1.00	37.28
763	CG	ARG	A	220	-5.058	35.372	87.750	1.00	44.07
764	CD	ARG	A	220	-3.665	35.138	87.075	1.00	53.39
765	NE	ARG	A	220	-3.131	36.401	86.587	1.00	57.56
766	CZ	ARG	A	220	-3.067	36.736	85.300	1.00	63.45
767	NH1	ARG	A	220	-2.583	37.921	84.937	1.00	62.86
768	NH2	ARG	A	220	-3.473	35.882	84.365	1.00	65.24
769	C	ARG	A	220	-7.561	37.846	87.621	1.00	35.84
770	O	ARG	A	220	-7.328	38.467	88.683	1.00	34.61
771	N	GLU	A	221	-7.928	38.427	86.490	1.00	35.98
772	CA	GLU	A	221	-8.145	39.852	86.355	1.00	38.35
773	CB	GLU	A	221	-8.573	40.154	84.930	1.00	39.07
774	CG	GLU	A	221	-8.452	41.597	84.521	1.00	47.19
775	CD	GLU	A	221	-7.205	42.221	85.080	1.00	57.25
776	OE1	GLU	A	221	-6.259	42.459	84.291	1.00	60.27
777	OE2	GLU	A	221	-7.178	42.474	86.314	1.00	62.91
778	C	GLU	A	221	-9.149	40.339	87.416	1.00	38.74
779	O	GLU	A	221	-8.832	41.307	88.117	1.00	38.67
780	N	LEU	A	222	-10.296	39.663	87.575	1.00	37.69
781	CA	LEU	A	222	-11.188	40.011	88.668	1.00	39.29
782	CB	LEU	A	222	-12.513	39.256	88.615	1.00	40.21
783	CG	LEU	A	222	-13.754	39.901	88.040	1.00	44.66
784	CD1	LEU	A	222	-13.892	41.386	88.378	1.00	44.76
785	CD2	LEU	A	222	-13.856	39.644	86.553	1.00	52.48
786	C	LEU	A	222	-10.654	39.766	90.079	1.00	40.79
787	O	LEU	A	222	-10.981	40.510	91.025	1.00	40.30
788	N	GLN	A	223	-9.904	38.712	90.272	1.00	40.08
789	CA	GLN	A	223	-9.456	38.509	91.612	1.00	43.39
790	CB	GLN	A	223	-9.120	37.025	91.889	1.00	44.71
791	CG	GLN	A	223	-7.754	36.535	91.538	1.00	49.87
792	CD	GLN	A	223	-7.627	34.996	91.712	1.00	56.56
793	OE1	GLN	A	223	-6.942	34.309	90.918	1.00	58.11
794	NE2	GLN	A	223	-8.286	34.460	92.747	1.00	58.77
795	C	GLN	A	223	-8.380	39.560	91.978	1.00	43.05
796	O	GLN	A	223	-8.307	39.976	93.113	1.00	43.64
797	N	LYS	A	224	-7.673	40.083	90.988	1.00	42.20
798	CA	LYS	A	224	-6.690	41.126	91.203	1.00	42.99
799	CB	LYS	A	224	-5.815	41.282	89.985	1.00	43.53
800	CG	LYS	A	224	-4.818	42.422	90.066	1.00	48.88
801	CD	LYS	A	224	-4.028	42.585	88.762	1.00	53.83
802	CE	LYS	A	224	-4.857	43.218	87.650	1.00	57.23
803	NZ	LYS	A	224	-4.028	43.546	86.442	1.00	60.62
804	C	LYS	A	224	-7.356	42.461	91.560	1.00	43.04
805	O	LYS	A	224	-7.042	43.032	92.599	1.00	42.77
806	N	LEU	A	225	-8.297	42.913	90.732	1.00	40.83
807	CA	LEU	A	225	-9.019	44.181	90.897	1.00	41.08

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
808	CB	LEU	A	225	-9.501	44.691	89.533	1.00	39.93
809	CG	LEU	A	225	-8.469	45.241	88.540	1.00	43.97
810	CD1	LEU	A	225	-9.133	45.930	87.345	1.00	46.75
811	CD2	LEU	A	225	-7.332	46.154	89.189	1.00	43.17
812	C	LEU	A	225	-10.254	44.157	91.818	1.00	40.68
813	O	LEU	A	225	-10.784	45.218	92.182	1.00	40.10
814	N	SER	A	226	-10.732	42.961	92.147	1.00	40.56
815	CA	SER	A	226	-11.977	42.780	92.913	1.00	41.73
816	CB	SER	A	226	-11.943	43.579	94.225	1.00	43.22
817	OG	SER	A	226	-12.999	43.112	95.048	1.00	50.73
818	C	SER	A	226	-13.295	43.050	92.126	1.00	40.15
819	O	SER	A	226	-14.238	42.256	92.215	1.00	40.02
820	N	LYS	A	227	-13.373	44.163	91.397	1.00	38.66
821	CA	LYS	A	227	-14.500	44.424	90.506	1.00	38.28
822	CB	LYS	A	227	-15.744	44.876	91.241	1.00	39.83
823	CG	LYS	A	227	-15.527	46.112	92.107	1.00	43.19
824	CD	LYS	A	227	-16.763	46.395	92.964	1.00	47.23
825	CE	LYS	A	227	-17.009	47.898	93.037	1.00	50.59
826	NZ	LYS	A	227	-15.847	48.527	93.755	1.00	50.07
827	C	LYS	A	227	-14.057	45.437	89.453	1.00	37.32
828	O	LYS	A	227	-13.032	46.114	89.637	1.00	35.43
829	N	PHE	A	228	-14.784	45.541	88.339	1.00	34.98
830	CA	PHE	A	228	-14.287	46.384	87.241	1.00	34.36
831	CB	PHE	A	228	-14.483	45.686	85.908	1.00	32.60
832	CG	PHE	A	228	-13.706	44.403	85.761	1.00	32.22
833	CD1	PHE	A	228	-12.556	44.214	86.480	1.00	30.96
834	CE1	PHE	A	228	-11.797	43.063	86.350	1.00	34.49
835	CZ	PHE	A	228	-12.178	42.076	85.495	1.00	33.23
836	CE2	PHE	A	228	-13.374	42.246	84.752	1.00	34.03
837	CD2	PHE	A	228	-14.105	43.409	84.862	1.00	33.41
838	C	PHE	A	228	-15.057	47.675	87.146	1.00	35.43
839	O	PHE	A	228	-16.228	47.733	87.549	1.00	34.99
840	N	ASP	A	229	-14.441	48.714	86.591	1.00	36.24
841	CA	ASP	A	229	-15.233	49.943	86.453	1.00	38.49
842	CB	ASP	A	229	-14.302	51.205	86.331	1.00	39.70
843	CG	ASP	A	229	-13.484	51.241	85.072	1.00	44.65
844	OD1	ASP	A	229	-13.729	50.465	84.121	1.00	47.75
845	OD2	ASP	A	229	-12.527	52.046	84.948	1.00	52.81
846	C	ASP	A	229	-16.211	49.721	85.300	1.00	37.35
847	O	ASP	A	229	-16.187	48.669	84.633	1.00	35.10
848	N	GLU	A	230	-17.038	50.715	85.027	1.00	37.87
849	CA	GLU	A	230	-18.077	50.513	84.040	1.00	37.66
850	CB	GLU	A	230	-19.054	51.668	84.115	1.00	39.25
851	CG	GLU	A	230	-19.840	51.650	85.412	1.00	42.58
852	CD	GLU	A	230	-21.045	52.566	85.320	1.00	49.54
853	OE1	GLU	A	230	-22.168	52.129	85.629	1.00	52.06
854	OE2	GLU	A	230	-20.868	53.740	84.896	1.00	52.95
855	C	GLU	A	230	-17.483	50.440	82.659	1.00	36.98
856	O	GLU	A	230	-18.015	49.782	81.767	1.00	34.19
857	N	GLN	A	231	-16.382	51.159	82.461	1.00	36.82
858	CA	GLN	A	231	-15.764	51.174	81.152	1.00	36.74

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
859	CB	GLN	A	231	-14.587	52.171	81.128	1.00	37.55
860	CG	GLN	A	231	-14.995	53.671	81.393	1.00	43.18
861	CD	GLN	A	231	-16.011	53.956	82.522	1.00	46.32
862	OE1	GLN	A	231	-15.731	53.743	83.729	1.00	42.61
863	NE2	GLN	A	231	-17.181	54.488	82.121	1.00	47.58
864	C	GLN	A	231	-15.212	49.784	80.817	1.00	35.85
865	O	GLN	A	231	-15.382	49.294	79.724	1.00	36.28
866	N	ARG	A	232	-14.495	49.186	81.746	1.00	33.62
867	CA	ARG	A	232	-13.858	47.928	81.426	1.00	33.95
868	CB	ARG	A	232	-12.832	47.530	82.509	1.00	33.54
869	CG	ARG	A	232	-12.260	46.109	82.347	1.00	36.13
870	CD	ARG	A	232	-11.433	45.610	83.520	1.00	40.91
871	NE	ARG	A	232	-10.425	46.602	83.868	1.00	49.70
872	CZ	ARG	A	232	-9.221	46.706	83.323	1.00	52.36
873	NH1	ARG	A	232	-8.817	45.862	82.371	1.00	53.98
874	NH2	ARG	A	232	-8.409	47.659	83.757	1.00	55.77
875	C	ARG	A	232	-14.931	46.853	81.238	1.00	31.99
876	O	ARG	A	232	-14.813	46.023	80.341	1.00	31.18
877	N	THR	A	233	-15.971	46.890	82.072	1.00	30.75
878	CA	THR	A	233	-17.071	45.931	82.002	1.00	30.48
879	CB	THR	A	233	-18.080	46.242	83.085	1.00	31.41
880	OG1	THR	A	233	-17.464	45.953	84.337	1.00	28.31
881	CG2	THR	A	233	-19.358	45.267	82.986	1.00	28.26
882	C	THR	A	233	-17.783	46.052	80.670	1.00	30.81
883	O	THR	A	233	-17.937	45.050	79.937	1.00	29.48
884	N	ALA	A	234	-18.283	47.261	80.402	1.00	30.12
885	CA	ALA	A	234	-18.959	47.533	79.118	1.00	30.91
886	CB	ALA	A	234	-19.319	48.998	78.963	1.00	29.68
887	C	ALA	A	234	-18.104	47.102	77.946	1.00	30.58
888	O	ALA	A	234	-18.611	46.555	76.947	1.00	31.37
889	N	THR	A	235	-16.815	47.389	78.028	1.00	30.80
890	CA	THR	A	235	-15.928	46.948	76.953	1.00	32.35
891	CB	THR	A	235	-14.533	47.546	77.129	1.00	32.78
892	OG1	THR	A	235	-14.654	48.951	77.006	1.00	34.77
893	CG2	THR	A	235	-13.580	47.153	75.967	1.00	34.42
894	C	THR	A	235	-15.860	45.400	76.799	1.00	32.27
895	O	THR	A	235	-16.000	44.850	75.656	1.00	31.74
896	N	TYR	A	236	-15.711	44.693	77.914	1.00	30.81
897	CA	TYR	A	236	-15.676	43.199	77.861	1.00	29.77
898	CB	TYR	A	236	-15.384	42.639	79.250	1.00	29.80
899	CG	TYR	A	236	-13.950	42.738	79.720	1.00	32.58
900	CD1	TYR	A	236	-12.913	42.926	78.818	1.00	33.58
901	CE1	TYR	A	236	-11.617	42.996	79.243	1.00	36.97
902	CZ	TYR	A	236	-11.324	42.872	80.601	1.00	36.77
903	OH	TYR	A	236	-10.025	42.971	81.016	1.00	37.51
904	CE2	TYR	A	236	-12.330	42.686	81.516	1.00	35.78
905	CD2	TYR	A	236	-13.643	42.634	81.065	1.00	36.22
906	C	TYR	A	236	-17.042	42.628	77.377	1.00	29.01
907	O	TYR	A	236	-17.103	41.680	76.632	1.00	29.48
908	N	ILE	A	237	-18.139	43.236	77.814	1.00	30.01
909	CA	ILE	A	237	-19.472	42.788	77.378	1.00	30.81

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
910	CB	ILE	A	237	-20.591	43.548	78.061	1.00	29.26
911	CG1	ILE	A	237	-20.580	43.141	79.541	1.00	31.33
912	CD1	ILE	A	237	-20.607	41.494	79.786	1.00	32.72
913	CG2	ILE	A	237	-21.938	43.089	77.553	1.00	30.76
914	C	ILE	A	237	-19.524	42.975	75.874	1.00	30.97
915	O	ILE	A	237	-20.024	42.110	75.165	1.00	28.59
916	N	THR	A	238	-19.071	44.126	75.413	1.00	29.66
917	CA	THR	A	238	-19.074	44.331	73.936	1.00	31.58
918	CB	THR	A	238	-18.483	45.699	73.600	1.00	30.71
919	OG1	THR	A	238	-19.345	46.681	74.169	1.00	33.26
920	CG2	THR	A	238	-18.547	45.948	72.092	1.00	36.01
921	C	THR	A	238	-18.279	43.281	73.177	1.00	31.08
922	O	THR	A	238	-18.744	42.785	72.179	1.00	31.90
923	N	GLU	A	239	-17.037	43.029	73.578	1.00	30.93
924	CA	GLU	A	239	-16.252	41.972	72.973	1.00	33.24
925	CB	GLU	A	239	-14.875	41.829	73.619	1.00	34.28
926	CG	GLU	A	239	-14.045	43.126	73.458	1.00	41.57
927	CD	GLU	A	239	-12.704	43.109	74.200	1.00	50.78
928	OE1	GLU	A	239	-11.654	43.089	73.518	1.00	59.72
929	OE2	GLU	A	239	-12.655	43.120	75.451	1.00	51.19
930	C	GLU	A	239	-16.947	40.625	72.977	1.00	32.47
931	O	GLU	A	239	-16.890	39.912	72.000	1.00	31.96
932	N	LEU	A	240	-17.585	40.307	74.093	1.00	31.66
933	CA	LEU	A	240	-18.252	39.033	74.293	1.00	32.00
934	CB	LEU	A	240	-18.793	38.941	75.749	1.00	32.28
935	CG	LEU	A	240	-17.918	38.368	76.879	1.00	38.51
936	CD1	LEU	A	240	-17.987	39.156	78.226	1.00	40.94
937	CD2	LEU	A	240	-18.427	36.978	77.180	1.00	46.36
938	C	LEU	A	240	-19.433	38.992	73.363	1.00	31.20
939	O	LEU	A	240	-19.674	37.997	72.730	1.00	30.06
940	N	ALA	A	241	-20.189	40.074	73.311	1.00	30.48
941	CA	ALA	A	241	-21.385	40.079	72.470	1.00	30.85
942	CB	ALA	A	241	-22.161	41.336	72.673	1.00	28.64
943	C	ALA	A	241	-21.046	39.875	70.996	1.00	32.63
944	O	ALA	A	241	-21.803	39.233	70.268	1.00	34.13
945	N	ASN	A	242	-19.946	40.476	70.547	1.00	32.98
946	CA	ASN	A	242	-19.501	40.301	69.176	1.00	34.79
947	CB	ASN	A	242	-18.342	41.225	68.806	1.00	35.05
948	CG	ASN	A	242	-18.735	42.668	68.801	1.00	37.46
949	OD1	ASN	A	242	-19.820	43.009	68.356	1.00	41.91
950	ND2	ASN	A	242	-17.838	43.531	69.270	1.00	36.72
951	C	ASN	A	242	-19.045	38.878	68.944	1.00	33.66
952	O	ASN	A	242	-19.384	38.322	67.926	1.00	34.14
953	N	ALA	A	243	-18.284	38.287	69.871	1.00	33.13
954	CA	ALA	A	243	-17.846	36.899	69.686	1.00	33.50
955	CB	ALA	A	243	-16.883	36.413	70.821	1.00	32.46
956	C	ALA	A	243	-19.100	36.026	69.596	1.00	33.00
957	O	ALA	A	243	-19.170	35.121	68.775	1.00	34.04
958	N	LEU	A	244	-20.063	36.281	70.460	1.00	32.30
959	CA	LEU	A	244	-21.290	35.495	70.486	1.00	34.17
960	CB	LEU	A	244	-22.109	35.794	71.761	1.00	32.72

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
961	CG	LEU	A	244	-21.487	35.248	73.091	1.00	33.90
962	CD1	LEU	A	244	-22.375	35.636	74.211	1.00	34.58
963	CD2	LEU	A	244	-21.346	33.731	73.053	1.00	36.04
964	C	LEU	A	244	-22.155	35.710	69.239	1.00	35.07
965	O	LEU	A	244	-22.795	34.770	68.771	1.00	35.54
966	N	SER	A	245	-22.205	36.935	68.736	1.00	36.14
967	CA	SER	A	245	-22.968	37.144	67.497	1.00	37.32
968	CB	SER	A	245	-22.881	38.566	66.993	1.00	36.71
969	OG	SER	A	245	-23.518	39.430	67.885	1.00	40.23
970	C	SER	A	245	-22.396	36.244	66.430	1.00	37.77
971	O	SER	A	245	-23.168	35.561	65.712	1.00	39.78
972	N	TYR	A	246	-21.062	36.236	66.324	1.00	36.62
973	CA	TYR	A	246	-20.388	35.397	65.334	1.00	36.75
974	CB	TYR	A	246	-18.867	35.666	65.303	1.00	35.63
975	CG	TYR	A	246	-18.040	34.768	64.415	1.00	36.74
976	CD1	TYR	A	246	-17.752	35.114	63.086	1.00	41.06
977	CE1	TYR	A	246	-16.991	34.283	62.293	1.00	40.63
978	CZ	TYR	A	246	-16.491	33.118	62.824	1.00	42.34
979	OH	TYR	A	246	-15.711	32.256	62.077	1.00	41.50
980	CE2	TYR	A	246	-16.782	32.766	64.151	1.00	40.05
981	CD2	TYR	A	246	-17.538	33.590	64.897	1.00	34.12
982	C	TYR	A	246	-20.730	33.925	65.554	1.00	36.80
983	O	TYR	A	246	-21.143	33.248	64.624	1.00	36.65
984	N	CYS	A	247	-20.608	33.425	66.778	1.00	36.48
985	CA	CYS	A	247	-21.015	32.049	67.085	1.00	36.90
986	CB	CYS	A	247	-20.803	31.722	68.595	1.00	37.60
987	SG	CYS	A	247	-19.067	31.666	69.093	1.00	42.84
988	C	CYS	A	247	-22.473	31.711	66.758	1.00	37.39
989	O	CYS	A	247	-22.746	30.672	66.121	1.00	37.58
990	N	HIS	A	248	-23.400	32.529	67.256	1.00	36.67
991	CA	HIS	A	248	-24.817	32.267	67.094	1.00	37.58
992	CB	HIS	A	248	-25.698	33.244	67.876	1.00	37.99
993	CG	HIS	A	248	-25.520	33.191	69.372	1.00	34.73
994	ND1	HIS	A	248	-26.053	34.149	70.204	1.00	36.33
995	CE1	HIS	A	248	-25.718	33.886	71.452	1.00	37.79
996	NE2	HIS	A	248	-24.957	32.807	71.458	1.00	33.84
997	CD2	HIS	A	248	-24.812	32.354	70.168	1.00	33.28
998	C	HIS	A	248	-25.189	32.338	65.601	1.00	39.08
999	O	HIS	A	248	-26.098	31.629	65.132	1.00	39.68
1000	N	SER	A	249	-24.443	33.132	64.854	1.00	39.67
1001	CA	SER	A	249	-24.748	33.244	63.437	1.00	41.50
1002	CB	SER	A	249	-23.805	34.207	62.715	1.00	40.00
1003	OG	SER	A	249	-22.561	33.599	62.481	1.00	41.00
1004	C	SER	A	249	-24.644	31.857	62.870	1.00	42.73
1005	O	SER	A	249	-25.312	31.550	61.894	1.00	43.62
1006	N	LYS	A	250	-23.799	31.026	63.476	1.00	43.39
1007	CA	LYS	A	250	-23.626	29.655	63.026	1.00	44.23
1008	CB	LYS	A	250	-22.163	29.299	63.057	1.00	45.26
1009	CG	LYS	A	250	-21.329	30.154	62.111	1.00	46.88
1010	CD	LYS	A	250	-19.847	29.989	62.369	1.00	46.41
1011	CE	LYS	A	250	-19.102	31.086	61.674	1.00	50.41

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
1012	NZ	LYS	A	250	-18.101	30.510	60.721	1.00	55.71
1013	C	LYS	A	250	-24.430	28.706	63.912	1.00	44.23
1014	O	LYS	A	250	-24.318	27.494	63.813	1.00	44.92
1015	N	ARG	A	251	-25.252	29.280	64.771	1.00	43.03
1016	CA	ARG	A	251	-26.013	28.499	65.722	1.00	43.09
1017	CB	ARG	A	251	-27.003	27.566	65.025	1.00	44.17
1018	CG	ARG	A	251	-28.079	28.334	64.298	1.00	48.00
1019	CD	ARG	A	251	-29.293	28.613	65.135	1.00	52.94
1020	NE	ARG	A	251	-30.316	27.613	64.935	1.00	57.46
1021	CZ	ARG	A	251	-31.409	27.504	65.694	1.00	59.77
1022	NH1	ARG	A	251	-32.301	26.573	65.421	1.00	58.50
1023	NH2	ARG	A	251	-31.617	28.329	66.721	1.00	60.29
1024	C	ARG	A	251	-25.133	27.719	66.694	1.00	40.87
1025	O	ARG	A	251	-25.579	26.725	67.287	1.00	41.62
1026	N	VAL	A	252	-23.890	28.136	66.866	1.00	38.05
1027	CA	VAL	A	252	-23.090	27.469	67.883	1.00	35.63
1028	CB	VAL	A	252	-21.605	27.579	67.574	1.00	36.71
1029	CG1	VAL	A	252	-20.757	27.253	68.833	1.00	36.16
1030	CG2	VAL	A	252	-21.267	26.671	66.408	1.00	32.96
1031	C	VAL	A	252	-23.398	28.171	69.217	1.00	35.05
1032	O	VAL	A	252	-23.342	29.421	69.278	1.00	34.28
1033	N	ILE	A	253	-23.751	27.394	70.238	1.00	34.78
1034	CA	ILE	A	253	-24.036	27.990	71.537	1.00	34.21
1035	CB	ILE	A	253	-25.528	27.772	72.035	1.00	36.92
1036	CG1	ILE	A	253	-26.008	26.317	72.080	1.00	34.92
1037	CD1	ILE	A	253	-27.473	26.046	72.506	1.00	33.07
1038	CG2	ILE	A	253	-26.490	28.538	71.085	1.00	39.25
1039	C	ILE	A	253	-22.899	27.570	72.441	1.00	32.53
1040	O	ILE	A	253	-22.459	26.397	72.378	1.00	32.33
1041	N	HIS	A	254	-22.352	28.508	73.234	1.00	30.81
1042	CA	HIS	A	254	-21.118	28.158	73.987	1.00	29.80
1043	CB	HIS	A	254	-20.268	29.410	74.275	1.00	29.82
1044	CG	HIS	A	254	-19.012	29.095	75.010	1.00	27.09
1045	ND1	HIS	A	254	-19.012	28.695	76.327	1.00	28.08
1046	CE1	HIS	A	254	-17.763	28.515	76.729	1.00	29.12
1047	NE2	HIS	A	254	-16.960	28.776	75.712	1.00	31.85
1048	CD2	HIS	A	254	-17.712	29.137	74.622	1.00	26.39
1049	C	HIS	A	254	-21.449	27.412	75.287	1.00	29.59
1050	O	HIS	A	254	-20.897	26.345	75.563	1.00	28.85
1051	N	ARG	A	255	-22.405	27.957	76.024	1.00	30.83
1052	CA	ARG	A	255	-22.920	27.309	77.234	1.00	30.64
1053	CB	ARG	A	255	-23.388	25.859	76.916	1.00	30.22
1054	CG	ARG	A	255	-24.321	25.716	75.687	1.00	32.25
1055	CD	ARG	A	255	-25.189	24.432	75.685	1.00	31.75
1056	NE	ARG	A	255	-24.362	23.256	75.649	1.00	30.77
1057	CZ	ARG	A	255	-24.820	22.017	75.669	1.00	31.35
1058	NH1	ARG	A	255	-26.095	21.798	75.751	1.00	31.83
1059	NH2	ARG	A	255	-23.977	21.003	75.617	1.00	33.16
1060	C	ARG	A	255	-21.983	27.279	78.449	1.00	31.38
1061	O	ARG	A	255	-22.363	26.734	79.477	1.00	32.65
1062	N	ASP	A	256	-20.758	27.768	78.356	1.00	31.39

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
1063	CA	ASP	A	256	-19.870	27.725	79.524	1.00	31.75
1064	CB	ASP	A	256	-18.964	26.468	79.453	1.00	33.11
1065	CG	ASP	A	256	-18.280	26.139	80.746	1.00	35.07
1066	OD1	ASP	A	256	-18.773	26.510	81.850	1.00	40.12
1067	OD2	ASP	A	256	-17.221	25.488	80.765	1.00	36.02
1068	C	ASP	A	256	-19.086	29.003	79.566	1.00	31.14
1069	O	ASP	A	256	-17.867	29.025	79.770	1.00	30.07
1070	N	ILE	A	257	-19.785	30.091	79.314	1.00	29.90
1071	CA	ILE	A	257	-19.166	31.390	79.385	1.00	32.07
1072	CB	ILE	A	257	-20.057	32.311	78.676	1.00	32.32
1073	CG1	ILE	A	257	-19.935	31.982	77.143	1.00	33.96
1074	CD1	ILE	A	257	-21.111	32.476	76.377	1.00	40.55
1075	CG2	ILE	A	257	-19.737	33.701	78.956	1.00	34.18
1076	C	ILE	A	257	-19.064	31.704	80.897	1.00	33.31
1077	O	ILE	A	257	-20.100	31.754	81.616	1.00	34.68
1078	N	LYS	A	258	-17.824	31.761	81.371	1.00	31.48
1079	CA	LYS	A	258	-17.519	32.187	82.750	1.00	30.84
1080	CB	LYS	A	258	-17.738	31.082	83.740	1.00	30.14
1081	CG	LYS	A	258	-16.926	29.870	83.529	1.00	34.40
1082	CD	LYS	A	258	-17.629	28.644	84.283	1.00	38.03
1083	CE	LYS	A	258	-16.742	27.431	84.270	1.00	41.53
1084	NZ	LYS	A	258	-17.580	26.165	84.236	1.00	42.89
1085	C	LYS	A	258	-16.097	32.737	82.755	1.00	30.04
1086	O	LYS	A	258	-15.324	32.537	81.785	1.00	26.95
1087	N	PRO	A	259	-15.775	33.505	83.792	1.00	28.33
1088	CA	PRO	A	259	-14.498	34.201	83.824	1.00	28.63
1089	CB	PRO	A	259	-14.480	34.892	85.200	1.00	27.18
1090	CG	PRO	A	259	-15.974	35.164	85.421	1.00	28.54
1091	CD	PRO	A	259	-16.648	33.843	84.942	1.00	29.43
1092	C	PRO	A	259	-13.330	33.301	83.615	1.00	27.22
1093	O	PRO	A	259	-12.411	33.740	82.963	1.00	28.73
1094	N	GLU	A	260	-13.331	32.086	84.121	1.00	27.82
1095	CA	GLU	A	260	-12.176	31.226	83.876	1.00	28.92
1096	CB	GLU	A	260	-12.107	30.028	84.836	1.00	31.10
1097	CG	GLU	A	260	-13.445	29.310	84.935	1.00	35.20
1098	CD	GLU	A	260	-14.340	29.861	86.098	1.00	44.01
1099	OE1	GLU	A	260	-14.462	29.148	87.133	1.00	49.68
1100	OE2	GLU	A	260	-14.908	30.985	86.003	1.00	33.54
1101	C	GLU	A	260	-12.027	30.755	82.420	1.00	28.10
1102	O	GLU	A	260	-10.957	30.265	82.068	1.00	29.64
1103	N	ASN	A	261	-13.012	30.991	81.567	1.00	26.88
1104	CA	ASN	A	261	-12.871	30.603	80.189	1.00	26.98
1105	CB	ASN	A	261	-14.077	29.731	79.753	1.00	26.91
1106	CG	ASN	A	261	-14.099	28.389	80.436	1.00	26.82
1107	OD1	ASN	A	261	-13.048	27.832	80.771	1.00	28.36
1108	ND2	ASN	A	261	-15.322	27.808	80.578	1.00	25.54
1109	C	ASN	A	261	-12.786	31.829	79.266	1.00	28.17
1110	O	ASN	A	261	-12.988	31.685	78.040	1.00	28.42
1111	N	LEU	A	262	-12.540	33.021	79.848	1.00	27.97
1112	CA	LEU	A	262	-12.454	34.254	79.091	1.00	28.33
1113	CB	LEU	A	262	-13.351	35.341	79.662	1.00	29.50



**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
1114	CG	LEU	A	262	-14.856	35.024	79.655	1.00	28.47
1115	CD1	LEU	A	262	-15.646	36.167	80.215	1.00	30.27
1116	CD2	LEU	A	262	-15.308	34.782	78.142	1.00	27.13
1117	C	LEU	A	262	-11.011	34.681	79.268	1.00	29.16
1118	O	LEU	A	262	-10.554	34.891	80.405	1.00	28.97
1119	N	LEU	A	263	-10.299	34.765	78.163	1.00	26.56
1120	CA	LEU	A	263	-8.869	34.988	78.194	1.00	28.18
1121	CB	LEU	A	263	-8.103	33.942	77.360	1.00	26.68
1122	CG	LEU	A	263	-8.452	32.452	77.583	1.00	29.56
1123	CD1	LEU	A	263	-7.487	31.481	76.825	1.00	30.33
1124	CD2	LEU	A	263	-8.272	32.171	79.060	1.00	34.69
1125	C	LEU	A	263	-8.574	36.382	77.619	1.00	29.97
1126	O	LEU	A	263	-9.416	37.002	76.966	1.00	29.84
1127	N	LEU	A	264	-7.378	36.850	77.904	1.00	30.85
1128	CA	LEU	A	264	-6.951	38.182	77.486	1.00	30.74
1129	CB	LEU	A	264	-6.721	39.079	78.732	1.00	30.19
1130	CG	LEU	A	264	-7.965	39.287	79.626	1.00	30.14
1131	CD1	LEU	A	264	-7.590	39.909	81.031	1.00	32.30
1132	CD2	LEU	A	264	-9.105	40.109	78.954	1.00	31.52
1133	C	LEU	A	264	-5.737	38.121	76.554	1.00	30.62
1134	O	LEU	A	264	-4.722	37.498	76.853	1.00	29.43
1135	N	GLY	A	265	-5.901	38.736	75.390	1.00	31.75
1136	CA	GLY	A	265	-4.858	38.816	74.396	1.00	33.01
1137	C	GLY	A	265	-3.830	39.883	74.737	1.00	34.94
1138	O	GLY	A	265	-3.969	40.574	75.751	1.00	34.96
1139	N	SER	A	266	-2.807	40.035	73.891	1.00	36.48
1140	CA	SER	A	266	-1.722	40.978	74.178	1.00	39.30
1141	CB	SER	A	266	-0.547	40.820	73.179	1.00	39.61
1142	OG	SER	A	266	-1.009	40.865	71.841	1.00	45.24
1143	C	SER	A	266	-2.195	42.443	74.287	1.00	39.68
1144	O	SER	A	266	-1.591	43.221	74.989	1.00	41.74
1145	N	ALA	A	267	-3.286	42.827	73.641	1.00	39.84
1146	CA	ALA	A	267	-3.757	44.193	73.821	1.00	40.82
1147	CB	ALA	A	267	-4.312	44.745	72.510	1.00	41.57
1148	C	ALA	A	267	-4.826	44.245	74.881	1.00	40.28
1149	O	ALA	A	267	-5.507	45.246	75.017	1.00	41.69
1150	N	GLY	A	268	-4.999	43.160	75.616	1.00	38.92
1151	CA	GLY	A	268	-6.066	43.099	76.605	1.00	39.91
1152	C	GLY	A	268	-7.440	42.772	76.035	1.00	39.16
1153	O	GLY	A	268	-8.421	42.894	76.749	1.00	39.70
1154	N	GLU	A	269	-7.525	42.328	74.781	1.00	37.55
1155	CA	GLU	A	269	-8.846	42.066	74.210	1.00	37.18
1156	CB	GLU	A	269	-8.844	42.024	72.686	1.00	36.91
1157	CG	GLU	A	269	-7.914	40.966	72.111	1.00	42.45
1158	CD	GLU	A	269	-6.497	41.495	71.931	1.00	48.18
1159	OE1	GLU	A	269	-5.789	41.696	72.951	1.00	49.56
1160	OE2	GLU	A	269	-6.122	41.758	70.767	1.00	54.50
1161	C	GLU	A	269	-9.323	40.711	74.736	1.00	34.23
1162	O	GLU	A	269	-8.556	39.821	74.981	1.00	32.16
1163	N	LEU	A	270	-10.611	40.599	74.889	1.00	33.25
1164	CA	LEU	A	270	-11.188	39.438	75.496	1.00	33.59

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
1165	CB	LEU	A	270	-12.532	39.836	76.065	1.00	33.76
1166	CG	LEU	A	270	-13.339	38.735	76.759	1.00	35.55
1167	CD1	LEU	A	270	-14.388	39.362	77.722	1.00	38.75
1168	CD2	LEU	A	270	-14.078	37.912	75.720	1.00	35.40
1169	C	LEU	A	270	-11.330	38.372	74.432	1.00	33.86
1170	O	LEU	A	270	-11.671	38.675	73.243	1.00	34.74
1171	N	LYS	A	271	-11.099	37.133	74.834	1.00	31.42
1172	CA	LYS	A	271	-11.191	35.979	73.930	1.00	31.29
1173	CB	LYS	A	271	-9.795	35.492	73.555	1.00	31.80
1174	CG	LYS	A	271	-9.128	36.524	72.537	1.00	35.49
1175	CD	LYS	A	271	-7.766	36.110	72.033	1.00	38.66
1176	CE	LYS	A	271	-7.165	37.192	71.120	1.00	39.08
1177	NZ	LYS	A	271	-7.494	36.998	69.682	1.00	42.36
1178	C	LYS	A	271	-11.994	34.844	74.605	1.00	29.90
1179	O	LYS	A	271	-11.668	34.417	75.687	1.00	30.82
1180	N	ILE	A	272	-13.062	34.408	73.997	1.00	29.63
1181	CA	ILE	A	272	-13.770	33.287	74.572	1.00	31.28
1182	CB	ILE	A	272	-15.251	33.238	74.154	1.00	32.97
1183	CG1	ILE	A	272	-15.867	31.943	74.660	1.00	34.14
1184	CD1	ILE	A	272	-17.133	32.166	75.428	1.00	41.15
1185	CG2	ILE	A	272	-15.415	33.105	72.693	1.00	36.72
1186	C	ILE	A	272	-12.981	32.023	74.227	1.00	29.77
1187	O	ILE	A	272	-12.487	31.888	73.131	1.00	29.32
1188	N	ALA	A	273	-12.833	31.121	75.199	1.00	29.03
1189	CA	ALA	A	273	-12.072	29.905	75.040	1.00	28.02
1190	CB	ALA	A	273	-10.720	30.027	75.796	1.00	25.93
1191	C	ALA	A	273	-12.890	28.757	75.639	1.00	28.47
1192	O	ALA	A	273	-14.008	28.975	76.165	1.00	29.27
1193	N	ASP	A	274	-12.329	27.558	75.567	1.00	28.32
1194	CA	ASP	A	274	-12.900	26.361	76.217	1.00	30.13
1195	CB	ASP	A	274	-12.994	26.548	77.752	1.00	28.19
1196	CG	ASP	A	274	-13.273	25.239	78.444	1.00	30.91
1197	OD1	ASP	A	274	-13.354	25.219	79.681	1.00	27.79
1198	OD2	ASP	A	274	-13.407	24.145	77.794	1.00	33.55
1199	C	ASP	A	274	-14.278	25.977	75.649	1.00	29.52
1200	O	ASP	A	274	-15.326	26.170	76.275	1.00	28.76
1201	N	PHE	A	275	-14.288	25.489	74.427	1.00	29.79
1202	CA	PHE	A	275	-15.564	25.206	73.796	1.00	31.48
1203	CB	PHE	A	275	-15.508	25.464	72.250	1.00	30.13
1204	CG	PHE	A	275	-15.621	26.887	71.890	1.00	30.02
1205	CD1	PHE	A	275	-14.605	27.761	72.243	1.00	30.82
1206	CE1	PHE	A	275	-14.705	29.121	71.908	1.00	31.65
1207	CZ	PHE	A	275	-15.847	29.599	71.217	1.00	30.66
1208	CE2	PHE	A	275	-16.846	28.718	70.853	1.00	28.29
1209	CD2	PHE	A	275	-16.707	27.356	71.175	1.00	28.74
1210	C	PHE	A	275	-16.042	23.793	74.019	1.00	31.32
1211	O	PHE	A	275	-16.874	23.333	73.263	1.00	33.58
1212	N	GLY	A	276	-15.542	23.128	75.050	1.00	32.57
1213	CA	GLY	A	276	-15.980	21.764	75.409	1.00	33.27
1214	C	GLY	A	276	-17.470	21.591	75.718	1.00	33.63
1215	O	GLY	A	276	-18.005	20.503	75.585	1.00	35.45

# FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1216	N	TRP	A	277	-18.168	22.649	76.085	1.00	32.48
1217	CA	TRP	A	277	-19.590	22.515	76.352	1.00	32.61
1218	CB	TRP	A	277	-19.996	23.356	77.571	1.00	31.90
1219	CG	TRP	A	277	-19.872	22.560	78.827	1.00	33.69
1220	CD1	TRP	A	277	-18.906	22.655	79.755	1.00	35.79
1221	NE1	TRP	A	277	-19.139	21.779	80.781	1.00	39.83
1222	CE2	TRP	A	277	-20.287	21.083	80.520	1.00	39.15
1223	CD2	TRP	A	277	-20.784	21.563	79.295	1.00	36.18
1224	CE3	TRP	A	277	-21.976	21.021	78.795	1.00	37.42
1225	CZ3	TRP	A	277	-22.625	19.991	79.531	1.00	40.23
1226	CH2	TRP	A	277	-22.103	19.550	80.772	1.00	36.38
1227	CZ2	TRP	A	277	-20.945	20.080	81.281	1.00	39.03
1228	C	TRP	A	277	-20.375	22.965	75.141	1.00	31.77
1229	O	TRP	A	277	-21.575	22.921	75.138	1.00	31.92
1230	N	SER	A	278	-19.701	23.425	74.102	1.00	30.59
1231	CA	SER	A	278	-20.489	23.978	73.041	1.00	32.01
1232	CB	SER	A	278	-19.643	24.889	72.181	1.00	32.28
1233	OG	SER	A	278	-18.600	24.165	71.545	1.00	37.30
1234	C	SER	A	278	-21.253	22.892	72.194	1.00	33.25
1235	O	SER	A	278	-20.861	21.734	72.149	1.00	34.86
1236	N	VAL	A	279	-22.353	23.307	71.560	1.00	34.55
1237	CA	VAL	A	279	-23.201	22.424	70.775	1.00	36.63
1238	CB	VAL	A	279	-24.238	21.763	71.710	1.00	36.03
1239	CG1	VAL	A	279	-25.173	22.788	72.273	1.00	35.73
1240	CG2	VAL	A	279	-24.920	20.585	71.018	1.00	38.77
1241	C	VAL	A	279	-23.873	23.260	69.702	1.00	36.61
1242	O	VAL	A	279	-23.927	24.488	69.850	1.00	35.60
1243	N	HIS	A	280	-24.438	22.679	68.636	1.00	37.41
1244	CA	HIS	A	280	-25.231	23.526	67.764	1.00	37.57
1245	CB	HIS	A	280	-25.245	22.996	66.333	1.00	39.08
1246	CG	HIS	A	280	-23.897	23.025	65.714	1.00	39.44
1247	ND1	HIS	A	280	-23.001	21.988	65.841	1.00	45.81
1248	CE1	HIS	A	280	-21.883	22.296	65.203	1.00	45.95
1249	NE2	HIS	A	280	-22.028	23.493	64.660	1.00	46.60
1250	CD2	HIS	A	280	-23.283	23.969	64.964	1.00	45.31
1251	C	HIS	A	280	-26.590	23.569	68.343	1.00	37.33
1252	O	HIS	A	280	-27.040	22.566	68.911	1.00	37.60
1253	N	ALA	A	281	-27.212	24.737	68.237	1.00	36.55
1254	CA	ALA	A	281	-28.494	25.000	68.825	1.00	38.46
1255	CB	ALA	A	281	-28.828	26.461	68.875	1.00	37.40
1256	C	ALA	A	281	-29.597	24.175	68.213	1.00	41.55
1257	O	ALA	A	281	-29.485	23.958	67.009	1.00	41.26
1258	N	PRO	A	282	-30.764	24.290	68.822	1.00	41.87
1259	CA	PRO	A	282	-31.606	23.344	69.535	1.00	41.68
1260	CB	PRO	A	282	-32.618	22.859	68.482	1.00	42.55
1261	CG	PRO	A	282	-32.233	23.675	67.281	1.00	41.31
1262	CD	PRO	A	282	-31.631	25.026	67.910	1.00	44.02
1263	C	PRO	A	282	-30.712	22.264	70.155	1.00	40.86
1264	O	PRO	A	282	-30.004	21.537	69.457	1.00	40.78
1265	N	SER	A	283	-30.704	22.233	71.483	1.00	38.89
1266	CA	SER	A	283	-30.011	21.158	72.148	1.00	39.04

### FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1267	CB	SER	A	283	-28.515	21.411	72.222	1.00	38.52
1268	OG	SER	A	283	-27.832	20.358	72.915	1.00	40.61
1269	C	SER	A	283	-30.549	20.857	73.526	1.00	39.37
1270	O	SER	A	283	-31.163	21.706	74.190	1.00	39.84
1271	N	SER	A	284	-30.310	19.641	73.955	1.00	39.43
1272	CA	SER	A	284	-30.584	19.299	75.314	1.00	41.76
1273	CB	SER	A	284	-31.245	17.940	75.356	1.00	43.22
1274	OG	SER	A	284	-32.242	17.954	76.372	1.00	47.58
1275	C	SER	A	284	-29.239	19.218	75.979	1.00	42.43
1276	O	SER	A	284	-28.205	19.677	75.432	1.00	43.18
1277	N	ARG	A	285	-29.226	18.626	77.161	1.00	42.91
1278	CA	ARG	A	285	-27.980	18.390	77.875	1.00	43.85
1279	CB	ARG	A	285	-27.914	19.247	79.145	1.00	43.75
1280	CG	ARG	A	285	-26.582	19.105	79.889	1.00	43.99
1281	CD	ARG	A	285	-26.415	20.119	81.009	1.00	45.74
1282	NE	ARG	A	285	-27.612	20.161	81.838	1.00	49.71
1283	CZ	ARG	A	285	-27.710	19.525	82.988	1.00	52.93
1284	NH1	ARG	A	285	-28.822	19.597	83.713	1.00	53.76
1285	NH2	ARG	A	285	-26.675	18.805	83.415	1.00	55.88
1286	C	ARG	A	285	-27.906	16.906	78.267	1.00	43.69
1287	O	ARG	A	285	-28.836	16.435	78.958	1.00	44.26
1288	N	THR	A	288	-25.116	15.611	79.501	1.00	47.82
1289	CA	THR	A	288	-23.866	15.594	80.345	1.00	48.76
1290	CB	THR	A	288	-22.675	16.360	79.646	1.00	48.89
1291	OG1	THR	A	288	-22.479	15.933	78.293	1.00	51.35
1292	CG2	THR	A	288	-21.345	16.015	80.297	1.00	47.79
1293	C	THR	A	288	-24.101	16.243	81.732	1.00	49.14
1294	O	THR	A	288	-24.852	17.214	81.851	1.00	47.49
1295	N	LEU	A	289	-23.443	15.702	82.757	1.00	50.43
1296	CA	LEU	A	289	-23.441	16.283	84.118	1.00	53.20
1297	CB	LEU	A	289	-22.802	15.267	85.056	1.00	53.63
1298	CG	LEU	A	289	-23.766	14.793	86.121	1.00	57.03
1299	CD1	LEU	A	289	-24.112	15.959	87.046	1.00	59.33
1300	CD2	LEU	A	289	-25.011	14.189	85.463	1.00	60.93
1301	C	LEU	A	289	-22.694	17.651	84.276	1.00	53.31
1302	O	LEU	A	289	-21.619	17.817	83.725	1.00	53.60
1303	N	CYS	A	290	-23.229	18.557	85.113	1.00	55.50
1304	CA	CYS	A	290	-22.752	19.970	85.335	1.00	57.08
1305	CB	CYS	A	290	-23.926	20.833	85.843	1.00	57.49
1306	SG	CYS	A	290	-25.205	21.169	84.585	1.00	64.10
1307	C	CYS	A	290	-21.426	20.313	86.110	1.00	56.52
1308	O	CYS	A	290	-20.448	19.597	85.933	1.00	57.86
1309	N	GLY	A	291	-21.379	21.417	86.898	1.00	55.52
1310	CA	GLY	A	291	-20.169	21.921	87.613	1.00	52.28
1311	C	GLY	A	291	-20.635	23.035	88.583	1.00	50.12
1312	O	GLY	A	291	-21.578	22.837	89.335	1.00	49.36
1313	N	THR	A	292	-20.005	24.208	88.624	1.00	47.90
1314	CA	THR	A	292	-20.610	25.273	89.444	1.00	44.87
1315	CB	THR	A	292	-19.672	26.461	89.703	1.00	47.07
1316	OG1	THR	A	292	-20.442	27.619	90.103	1.00	47.16
1317	CG2	THR	A	292	-19.180	26.950	88.383	1.00	48.62

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
1318	C	THR	A	292	-21.798	25.781	88.602	1.00	41.88
1319	O	THR	A	292	-21.634	25.980	87.395	1.00	41.81
1320	N	LEU	A	293	-22.964	26.018	89.200	1.00	36.57
1321	CA	LEU	A	293	-24.101	26.475	88.391	1.00	35.69
1322	CB	LEU	A	293	-25.398	26.116	89.074	1.00	35.41
1323	CG	LEU	A	293	-26.168	24.807	88.850	1.00	42.89
1324	CD1	LEU	A	293	-25.377	23.623	88.364	1.00	43.78
1325	CD2	LEU	A	293	-27.014	24.434	90.111	1.00	43.98
1326	C	LEU	A	293	-24.158	27.975	88.146	1.00	33.14
1327	O	LEU	A	293	-25.017	28.435	87.395	1.00	32.15
1328	N	ASP	A	294	-23.246	28.729	88.755	1.00	31.34
1329	CA	ASP	A	294	-23.362	30.191	88.780	1.00	30.17
1330	CB	ASP	A	294	-22.072	30.788	89.362	1.00	31.41
1331	CG	ASP	A	294	-22.096	30.775	90.875	1.00	36.52
1332	OD1	ASP	A	294	-21.149	30.228	91.449	1.00	42.47
1333	OD2	ASP	A	294	-23.074	31.224	91.535	1.00	39.71
1334	C	ASP	A	294	-23.740	30.941	87.510	1.00	29.90
1335	O	ASP	A	294	-24.404	31.966	87.568	1.00	28.82
1336	N	TYR	A	295	-23.192	30.486	86.390	1.00	28.35
1337	CA	TYR	A	295	-23.409	31.144	85.110	1.00	29.18
1338	CB	TYR	A	295	-22.081	31.134	84.392	1.00	29.58
1339	CG	TYR	A	295	-21.064	31.857	85.196	1.00	28.98
1340	CD1	TYR	A	295	-20.229	31.183	86.080	1.00	33.43
1341	CE1	TYR	A	295	-19.281	31.854	86.858	1.00	35.92
1342	CZ	TYR	A	295	-19.257	33.216	86.782	1.00	33.99
1343	OH	TYR	A	295	-18.331	33.880	87.548	1.00	39.27
1344	CE2	TYR	A	295	-20.078	33.903	85.910	1.00	33.69
1345	CD2	TYR	A	295	-20.983	33.215	85.124	1.00	32.42
1346	C	TYR	A	295	-24.468	30.562	84.180	1.00	30.12
1347	O	TYR	A	295	-24.606	31.005	83.032	1.00	29.57
1348	N	LEU	A	296	-25.192	29.556	84.637	1.00	29.88
1349	CA	LEU	A	296	-26.160	28.872	83.753	1.00	30.57
1350	CB	LEU	A	296	-26.090	27.394	83.996	1.00	31.08
1351	CG	LEU	A	296	-24.686	26.827	83.787	1.00	36.71
1352	CD1	LEU	A	296	-24.675	25.310	84.148	1.00	38.55
1353	CD2	LEU	A	296	-24.209	27.111	82.373	1.00	35.88
1354	C	LEU	A	296	-27.547	29.301	84.042	1.00	30.06
1355	O	LEU	A	296	-27.902	29.441	85.223	1.00	28.76
1356	N	PRO	A	297	-28.346	29.432	82.969	1.00	29.59
1357	CA	PRO	A	297	-29.752	29.814	83.035	1.00	29.63
1358	CB	PRO	A	297	-30.105	30.142	81.563	1.00	30.10
1359	CG	PRO	A	297	-29.256	29.232	80.816	1.00	30.36
1360	CD	PRO	A	297	-27.902	29.176	81.578	1.00	30.37
1361	C	PRO	A	297	-30.593	28.606	83.518	1.00	30.53
1362	O	PRO	A	297	-30.133	27.475	83.493	1.00	29.72
1363	N	PRO	A	298	-31.785	28.907	83.980	1.00	32.38
1364	CA	PRO	A	298	-32.748	27.911	84.486	1.00	35.25
1365	CB	PRO	A	298	-34.030	28.716	84.623	1.00	34.69
1366	CG	PRO	A	298	-33.555	30.121	84.897	1.00	35.48
1367	CD	PRO	A	298	-32.269	30.280	84.096	1.00	32.59
1368	C	PRO	A	298	-32.951	26.766	83.492	1.00	37.27

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
1369	O	PRO	A	298	-32.829	25.611	83.920	1.00	38.20
1370	N	GLU	A	299	-33.089	27.056	82.197	1.00	38.20
1371	CA	GLU	A	299	-33.396	25.984	81.252	1.00	40.09
1372	CB	GLU	A	299	-33.745	26.499	79.833	1.00	39.94
1373	CG	GLU	A	299	-32.614	27.242	79.139	1.00	39.16
1374	CD	GLU	A	299	-32.578	28.754	79.410	1.00	39.82
1375	OE1	GLU	A	299	-33.124	29.242	80.436	1.00	37.57
1376	OE2	GLU	A	299	-31.980	29.467	78.564	1.00	37.07
1377	C	GLU	A	299	-32.299	24.969	81.174	1.00	41.23
1378	O	GLU	A	299	-32.543	23.747	81.097	1.00	41.06
1379	N	MET	A	300	-31.075	25.468	81.248	1.00	41.85
1380	CA	MET	A	300	-29.951	24.596	81.206	1.00	43.22
1381	CB	MET	A	300	-28.679	25.376	81.027	1.00	43.88
1382	CG	MET	A	300	-27.499	24.515	81.020	1.00	49.44
1383	SD	MET	A	300	-26.839	24.501	79.396	1.00	60.26
1384	CE	MET	A	300	-25.544	23.343	79.572	1.00	54.71
1385	C	MET	A	300	-29.837	23.750	82.461	1.00	44.15
1386	O	MET	A	300	-29.682	22.512	82.356	1.00	44.33
1387	N	ILE	A	301	-29.864	24.362	83.638	1.00	44.85
1388	CA	ILE	A	301	-29.735	23.521	84.831	1.00	46.79
1389	CB	ILE	A	301	-29.657	24.332	86.111	1.00	47.71
1390	CG1	ILE	A	301	-30.818	25.308	86.276	1.00	50.37
1391	CD1	ILE	A	301	-30.163	26.709	86.641	1.00	56.06
1392	CG2	ILE	A	301	-28.369	25.222	86.119	1.00	46.42
1393	C	ILE	A	301	-30.836	22.441	84.891	1.00	48.14
1394	O	ILE	A	301	-30.538	21.258	85.093	1.00	48.00
1395	N	GLU	A	302	-32.085	22.854	84.677	1.00	49.20
1396	CA	GLU	A	302	-33.236	21.952	84.671	1.00	51.02
1397	CB	GLU	A	302	-34.520	22.754	84.559	1.00	51.41
1398	CG	GLU	A	302	-34.831	23.576	85.792	1.00	55.27
1399	CD	GLU	A	302	-35.798	24.695	85.474	1.00	59.81
1400	OE1	GLU	A	302	-36.087	25.555	86.349	1.00	63.64
1401	OE2	GLU	A	302	-36.294	24.693	84.335	1.00	60.77
1402	C	GLU	A	302	-33.242	20.937	83.540	1.00	51.10
1403	O	GLU	A	302	-34.179	20.143	83.434	1.00	51.91
1404	N	GLY	A	303	-32.240	20.988	82.669	1.00	50.72
1405	CA	GLY	A	303	-32.155	20.071	81.553	1.00	49.63
1406	C	GLY	A	303	-33.262	20.211	80.509	1.00	49.30
1407	O	GLY	A	303	-33.624	19.227	79.864	1.00	50.60
1408	N	ARG	A	304	-33.809	21.402	80.323	1.00	47.24
1409	CA	ARG	A	304	-34.799	21.609	79.256	1.00	46.04
1410	CB	ARG	A	304	-35.716	22.800	79.591	1.00	46.73
1411	CG	ARG	A	304	-36.712	22.504	80.773	1.00	49.63
1412	CD	ARG	A	304	-37.419	23.759	81.406	1.00	55.75
1413	NE	ARG	A	304	-37.497	24.898	80.477	1.00	58.41
1414	CZ	ARG	A	304	-37.277	26.172	80.822	1.00	60.70
1415	NH1	ARG	A	304	-37.360	27.151	79.903	1.00	61.20
1416	NH2	ARG	A	304	-36.965	26.473	82.083	1.00	58.65
1417	C	ARG	A	304	-34.097	21.838	77.907	1.00	44.67
1418	O	ARG	A	304	-32.861	21.996	77.852	1.00	43.50
1419	N	MET	A	305	-34.858	21.822	76.819	1.00	41.82

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
1420	CA	MET	A	305	-34.254	22.089	75.503	1.00	42.19
1421	CB	MET	A	305	-35.229	21.851	74.333	1.00	41.21
1422	CG	MET	A	305	-35.426	20.357	73.940	1.00	49.17
1423	SD	MET	A	305	-33.904	19.263	73.897	1.00	58.33
1424	CE	MET	A	305	-33.530	19.109	72.178	1.00	55.74
1425	C	MET	A	305	-33.865	23.563	75.506	1.00	38.86
1426	O	MET	A	305	-34.562	24.353	76.091	1.00	38.98
1427	N	HIS	A	306	-32.786	23.933	74.838	1.00	37.11
1428	CA	HIS	A	306	-32.358	25.332	74.903	1.00	36.23
1429	CB	HIS	A	306	-31.486	25.515	76.164	1.00	34.70
1430	CG	HIS	A	306	-30.350	24.541	76.239	1.00	31.57
1431	ND1	HIS	A	306	-30.436	23.353	76.920	1.00	30.19
1432	CE1	HIS	A	306	-29.306	22.688	76.809	1.00	31.98
1433	NE2	HIS	A	306	-28.485	23.405	76.061	1.00	33.02
1434	CD2	HIS	A	306	-29.117	24.569	75.698	1.00	31.19
1435	C	HIS	A	306	-31.570	25.711	73.662	1.00	36.80
1436	O	HIS	A	306	-31.106	24.834	72.897	1.00	36.60
1437	N	ASP	A	307	-31.378	27.017	73.498	1.00	37.06
1438	CA	ASP	A	307	-30.728	27.538	72.310	1.00	37.90
1439	CB	ASP	A	307	-31.778	27.990	71.294	1.00	38.38
1440	CG	ASP	A	307	-32.671	29.159	71.810	1.00	43.93
1441	OD1	ASP	A	307	-33.590	29.626	71.077	1.00	51.28
1442	OD2	ASP	A	307	-32.554	29.695	72.926	1.00	43.92
1443	C	ASP	A	307	-29.824	28.702	72.622	1.00	37.59
1444	O	ASP	A	307	-29.361	28.848	73.739	1.00	37.38
1445	N	GLU	A	308	-29.676	29.585	71.642	1.00	36.80
1446	CA	GLU	A	308	-28.726	30.683	71.742	1.00	37.37
1447	CB	GLU	A	308	-28.825	31.551	70.492	1.00	37.85
1448	CG	GLU	A	308	-28.228	30.905	69.266	1.00	40.29
1449	CD	GLU	A	308	-29.197	29.990	68.528	1.00	45.91
1450	OE1	GLU	A	308	-30.253	29.629	69.089	1.00	43.52
1451	OE2	GLU	A	308	-28.879	29.616	67.361	1.00	48.59
1452	C	GLU	A	308	-29.008	31.574	72.946	1.00	35.64
1453	O	GLU	A	308	-28.099	32.237	73.434	1.00	34.56
1454	N	LYS	A	309	-30.247	31.603	73.410	1.00	33.77
1455	CA	LYS	A	309	-30.557	32.491	74.535	1.00	33.68
1456	CB	LYS	A	309	-32.071	32.589	74.813	1.00	34.13
1457	CG	LYS	A	309	-32.853	33.190	73.626	1.00	35.58
1458	CD	LYS	A	309	-32.289	34.571	73.302	1.00	39.16
1459	CE	LYS	A	309	-33.289	35.387	72.485	1.00	46.27
1460	NZ	LYS	A	309	-34.624	35.259	73.121	1.00	46.60
1461	C	LYS	A	309	-29.793	32.123	75.816	1.00	32.90
1462	O	LYS	A	309	-29.673	32.945	76.708	1.00	32.40
1463	N	VAL	A	310	-29.242	30.932	75.870	1.00	31.17
1464	CA	VAL	A	310	-28.473	30.508	77.022	1.00	32.76
1465	CB	VAL	A	310	-27.993	29.086	76.822	1.00	33.19
1466	CG1	VAL	A	310	-26.762	28.825	77.639	1.00	36.49
1467	CG2	VAL	A	310	-29.154	28.095	77.249	1.00	32.68
1468	C	VAL	A	310	-27.292	31.457	77.250	1.00	33.09
1469	O	VAL	A	310	-27.083	31.951	78.365	1.00	31.77
1470	N	ASP	A	311	-26.568	31.770	76.175	1.00	31.32

### FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1471	CA	ASP	A	311	-25.422	32.682	76.275	1.00	32.19
1472	CB	ASP	A	311	-24.578	32.656	74.950	1.00	32.21
1473	CG	ASP	A	311	-23.893	31.256	74.696	1.00	33.63
1474	OD1	ASP	A	311	-23.601	30.482	75.635	1.00	34.07
1475	OD2	ASP	A	311	-23.615	30.806	73.584	1.00	34.64
1476	C	ASP	A	311	-25.848	34.089	76.674	1.00	31.34
1477	O	ASP	A	311	-25.054	34.819	77.265	1.00	31.50
1478	N	LEU	A	312	-27.074	34.500	76.349	1.00	30.65
1479	CA	LEU	A	312	-27.540	35.829	76.741	1.00	30.65
1480	CB	LEU	A	312	-28.880	36.194	76.114	1.00	32.89
1481	CG	LEU	A	312	-28.740	36.747	74.676	1.00	33.15
1482	CD1	LEU	A	312	-27.998	38.080	74.782	1.00	37.24
1483	CD2	LEU	A	312	-27.978	35.740	73.770	1.00	37.98
1484	C	LEU	A	312	-27.659	35.915	78.252	1.00	30.10
1485	O	LEU	A	312	-27.212	36.882	78.870	1.00	29.74
1486	N	TRP	A	313	-28.221	34.878	78.847	1.00	28.70
1487	CA	TRP	A	313	-28.290	34.885	80.311	1.00	29.18
1488	CB	TRP	A	313	-28.980	33.655	80.774	1.00	29.28
1489	CG	TRP	A	313	-28.856	33.398	82.197	1.00	29.13
1490	CD1	TRP	A	313	-27.798	32.871	82.848	1.00	26.72
1491	NE1	TRP	A	313	-28.104	32.728	84.184	1.00	28.25
1492	CE2	TRP	A	313	-29.402	33.129	84.370	1.00	28.86
1493	CD2	TRP	A	313	-29.877	33.584	83.145	1.00	26.93
1494	CE3	TRP	A	313	-31.192	34.028	83.062	1.00	26.93
1495	CZ3	TRP	A	313	-31.969	34.038	84.199	1.00	31.77
1496	CH2	TRP	A	313	-31.450	33.635	85.422	1.00	28.09
1497	CZ2	TRP	A	313	-30.175	33.170	85.538	1.00	26.06
1498	C	TRP	A	313	-26.880	34.959	80.918	1.00	29.84
1499	O	TRP	A	313	-26.633	35.738	81.823	1.00	27.08
1500	N	SER	A	314	-25.958	34.152	80.409	1.00	29.72
1501	CA	SER	A	314	-24.593	34.162	80.901	1.00	30.37
1502	CB	SER	A	314	-23.777	33.087	80.139	1.00	30.46
1503	OG	SER	A	314	-24.244	31.776	80.494	1.00	35.30
1504	C	SER	A	314	-23.937	35.568	80.801	1.00	31.13
1505	O	SER	A	314	-23.199	35.980	81.679	1.00	27.77
1506	N	LEU	A	315	-24.183	36.276	79.708	1.00	30.52
1507	CA	LEU	A	315	-23.699	37.630	79.537	1.00	31.47
1508	CB	LEU	A	315	-24.303	38.182	78.258	1.00	31.92
1509	CG	LEU	A	315	-23.556	39.322	77.630	1.00	34.89
1510	CD1	LEU	A	315	-22.077	38.966	77.617	1.00	32.65
1511	CD2	LEU	A	315	-24.094	39.490	76.207	1.00	34.24
1512	C	LEU	A	315	-24.189	38.521	80.657	1.00	30.26
1513	O	LEU	A	315	-23.467	39.375	81.154	1.00	29.93
1514	N	GLY	A	316	-25.416	38.270	81.084	1.00	31.24
1515	CA	GLY	A	316	-26.030	39.018	82.160	1.00	28.40
1516	C	GLY	A	316	-25.336	38.709	83.470	1.00	29.31
1517	O	GLY	A	316	-24.989	39.635	84.232	1.00	28.62
1518	N	VAL	A	317	-25.123	37.426	83.751	1.00	29.39
1519	CA	VAL	A	317	-24.392	37.045	84.964	1.00	29.86
1520	CB	VAL	A	317	-24.272	35.498	85.118	1.00	29.69
1521	CG1	VAL	A	317	-23.433	35.135	86.302	1.00	31.40



**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
1522	CG2	VAL	A	317	-25.625	34.885	85.201	1.00	30.52
1523	C	VAL	A	317	-22.971	37.715	84.961	1.00	30.09
1524	O	VAL	A	317	-22.525	38.275	85.976	1.00	28.93
1525	N	LEU	A	318	-22.283	37.665	83.832	1.00	29.07
1526	CA	LEU	A	318	-20.973	38.219	83.759	1.00	29.74
1527	CB	LEU	A	318	-20.327	37.940	82.391	1.00	29.62
1528	CG	LEU	A	318	-19.795	36.566	82.116	1.00	33.45
1529	CD1	LEU	A	318	-19.343	36.587	80.606	1.00	31.59
1530	CD2	LEU	A	318	-18.570	36.186	83.001	1.00	26.99
1531	C	LEU	A	318	-21.015	39.716	83.938	1.00	29.78
1532	O	LEU	A	318	-20.140	40.243	84.572	1.00	29.27
1533	N	CYS	A	319	-22.036	40.401	83.423	1.00	29.91
1534	CA	CYS	A	319	-22.072	41.831	83.606	1.00	31.51
1535	CB	CYS	A	319	-23.214	42.431	82.818	1.00	31.68
1536	SG	CYS	A	319	-23.007	44.241	82.719	1.00	40.49
1537	C	CYS	A	319	-22.152	42.216	85.116	1.00	31.22
1538	O	CYS	A	319	-21.439	43.092	85.632	1.00	29.46
1539	N	TYR	A	320	-22.985	41.482	85.819	1.00	29.74
1540	CA	TYR	A	320	-23.149	41.689	87.243	1.00	28.88
1541	CB	TYR	A	320	-24.320	40.843	87.746	1.00	28.54
1542	CG	TYR	A	320	-24.606	40.973	89.212	1.00	28.67
1543	CD1	TYR	A	320	-23.746	40.436	90.152	1.00	28.63
1544	CE1	TYR	A	320	-24.037	40.574	91.521	1.00	31.25
1545	CZ	TYR	A	320	-25.218	41.261	91.901	1.00	27.73
1546	OH	TYR	A	320	-25.601	41.384	93.204	1.00	34.97
1547	CE2	TYR	A	320	-26.070	41.711	91.016	1.00	28.41
1548	CD2	TYR	A	320	-25.745	41.625	89.636	1.00	27.53
1549	C	TYR	A	320	-21.810	41.373	87.977	1.00	29.65
1550	O	TYR	A	320	-21.286	42.208	88.741	1.00	28.99
1551	N	GLU	A	321	-21.252	40.185	87.727	1.00	28.26
1552	CA	GLU	A	321	-19.996	39.790	88.381	1.00	29.29
1553	CB	GLU	A	321	-19.511	38.398	87.976	1.00	27.46
1554	CG	GLU	A	321	-18.367	37.989	88.874	1.00	31.39
1555	CD	GLU	A	321	-17.939	36.565	88.757	1.00	39.04
1556	OE1	GLU	A	321	-16.893	36.204	89.386	1.00	40.16
1557	OE2	GLU	A	321	-18.629	35.792	88.062	1.00	41.43
1558	C	GLU	A	321	-18.858	40.810	88.173	1.00	29.09
1559	O	GLU	A	321	-18.148	41.162	89.112	1.00	28.70
1560	N	PHE	A	322	-18.712	41.290	86.942	1.00	28.18
1561	CA	PHE	A	322	-17.690	42.282	86.620	1.00	29.59
1562	CB	PHE	A	322	-17.742	42.671	85.130	1.00	30.02
1563	CG	PHE	A	322	-17.277	41.578	84.189	1.00	29.13
1564	CD1	PHE	A	322	-16.706	40.416	84.659	1.00	29.70
1565	CE1	PHE	A	322	-16.287	39.422	83.772	1.00	32.17
1566	CZ	PHE	A	322	-16.416	39.619	82.418	1.00	33.54
1567	CE2	PHE	A	322	-16.981	40.753	81.954	1.00	33.04
1568	CD2	PHE	A	322	-17.412	41.738	82.844	1.00	30.45
1569	C	PHE	A	322	-17.874	43.526	87.468	1.00	30.51
1570	O	PHE	A	322	-16.924	44.017	88.092	1.00	32.18
1571	N	LEU	A	323	-19.079	44.047	87.443	1.00	30.76
1572	CA	LEU	A	323	-19.461	45.235	88.188	1.00	31.93

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
1573	CB	LEU	A	323	-20.850	45.703	87.765	1.00	31.23
1574	CG	LEU	A	323	-21.005	46.300	86.372	1.00	29.55
1575	CD1	LEU	A	323	-22.381	46.696	86.162	1.00	28.14
1576	CD2	LEU	A	323	-20.049	47.538	86.199	1.00	33.58
1577	C	LEU	A	323	-19.455	45.015	89.689	1.00	33.43
1578	O	LEU	A	323	-19.064	45.912	90.469	1.00	33.54
1579	N	VAL	A	324	-19.868	43.827	90.139	1.00	33.63
1580	CA	VAL	A	324	-20.061	43.630	91.587	1.00	33.28
1581	CB	VAL	A	324	-21.449	42.976	91.860	1.00	33.80
1582	CG1	VAL	A	324	-21.709	42.622	93.380	1.00	32.67
1583	CG2	VAL	A	324	-22.586	43.857	91.300	1.00	34.21
1584	C	VAL	A	324	-18.928	42.911	92.263	1.00	35.51
1585	O	VAL	A	324	-18.642	43.145	93.424	1.00	35.39
1586	N	GLY	A	325	-18.226	42.038	91.560	1.00	35.56
1587	CA	GLY	A	325	-17.194	41.273	92.225	1.00	35.35
1588	C	GLY	A	325	-17.594	39.835	92.535	1.00	36.00
1589	O	GLY	A	325	-16.746	39.003	92.813	1.00	37.09
1590	N	LYS	A	326	-18.880	39.528	92.442	1.00	35.21
1591	CA	LYS	A	326	-19.304	38.161	92.638	1.00	35.82
1592	CB	LYS	A	326	-19.650	37.922	94.122	1.00	35.98
1593	CG	LYS	A	326	-20.941	38.598	94.489	1.00	40.08
1594	CD	LYS	A	326	-21.233	38.587	96.024	1.00	47.40
1595	CE	LYS	A	326	-22.214	39.748	96.321	1.00	51.86
1596	NZ	LYS	A	326	-21.819	40.553	97.484	1.00	48.80
1597	C	LYS	A	326	-20.512	37.929	91.754	1.00	33.85
1598	O	LYS	A	326	-21.227	38.853	91.451	1.00	31.55
1599	N	PRO	A	327	-20.755	36.691	91.332	1.00	33.50
1600	CA	PRO	A	327	-21.927	36.437	90.463	1.00	32.79
1601	CB	PRO	A	327	-21.678	34.994	89.969	1.00	33.94
1602	CG	PRO	A	327	-21.026	34.347	91.241	1.00	35.31
1603	CD	PRO	A	327	-19.983	35.449	91.621	1.00	33.33
1604	C	PRO	A	327	-23.245	36.595	91.255	1.00	30.81
1605	O	PRO	A	327	-23.300	36.380	92.463	1.00	32.11
1606	N	PRO	A	328	-24.309	36.989	90.598	1.00	29.67
1607	CA	PRO	A	328	-25.541	37.336	91.315	1.00	29.91
1608	CB	PRO	A	328	-26.396	37.936	90.249	1.00	28.24
1609	CG	PRO	A	328	-25.879	37.253	88.972	1.00	30.64
1610	CD	PRO	A	328	-24.406	37.239	89.158	1.00	29.03
1611	C	PRO	A	328	-26.291	36.189	92.066	1.00	32.07
1612	O	PRO	A	328	-27.110	36.498	92.935	1.00	31.51
1613	N	PHE	A	329	-26.007	34.919	91.745	1.00	30.77
1614	CA	PHE	A	329	-26.723	33.835	92.391	1.00	32.15
1615	CB	PHE	A	329	-27.367	32.923	91.329	1.00	30.34
1616	CG	PHE	A	329	-28.198	33.663	90.371	1.00	29.16
1617	CD1	PHE	A	329	-29.349	34.294	90.783	1.00	26.86
1618	CE1	PHE	A	329	-30.109	35.003	89.921	1.00	26.79
1619	CZ	PHE	A	329	-29.692	35.115	88.583	1.00	29.19
1620	CE2	PHE	A	329	-28.507	34.503	88.156	1.00	28.24
1621	CD2	PHE	A	329	-27.779	33.782	89.042	1.00	29.12
1622	C	PHE	A	329	-25.833	33.027	93.287	1.00	33.34
1623	O	PHE	A	329	-26.260	31.988	93.763	1.00	35.58

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
1624	N	GLU	A	330	-24.623	33.505	93.513	1.00	35.42
1625	CA	GLU	A	330	-23.656	32.877	94.397	1.00	38.76
1626	CB	GLU	A	330	-22.588	33.906	94.768	1.00	39.72
1627	CG	GLU	A	330	-21.251	33.325	95.177	1.00	44.21
1628	CD	GLU	A	330	-20.378	34.364	95.894	1.00	53.19
1629	OE1	GLU	A	330	-20.779	34.883	96.993	1.00	53.55
1630	OE2	GLU	A	330	-19.295	34.665	95.337	1.00	58.16
1631	C	GLU	A	330	-24.373	32.498	95.704	1.00	39.04
1632	O	GLU	A	330	-25.175	33.269	96.217	1.00	37.84
1633	N	ALA	A	331	-24.084	31.303	96.200	1.00	40.28
1634	CA	ALA	A	331	-24.680	30.771	97.425	1.00	40.27
1635	CB	ALA	A	331	-26.002	30.149	97.126	1.00	41.00
1636	C	ALA	A	331	-23.658	29.753	97.888	1.00	41.45
1637	O	ALA	A	331	-22.757	29.404	97.127	1.00	41.16
1638	N	ASN	A	332	-23.776	29.280	99.121	1.00	41.89
1639	CA	ASN	A	332	-22.737	28.404	99.662	1.00	40.88
1640	CB	ASN	A	332	-22.602	28.566	101.220	1.00	43.11
1641	CG	ASN	A	332	-21.784	29.826	101.626	1.00	48.66
1642	OD1	ASN	A	332	-20.570	29.937	101.359	1.00	55.22
1643	ND2	ASN	A	332	-22.462	30.786	102.245	1.00	55.15
1644	C	ASN	A	332	-23.050	26.959	99.235	1.00	37.57
1645	O	ASN	A	332	-22.225	26.050	99.332	1.00	39.59
1646	N	THR	A	333	-24.231	26.755	98.724	1.00	36.44
1647	CA	THR	A	333	-24.536	25.410	98.298	1.00	36.73
1648	CB	THR	A	333	-25.645	24.665	99.264	1.00	37.09
1649	OG1	THR	A	333	-25.097	24.779	100.596	1.00	40.58
1650	CG2	THR	A	333	-25.650	23.188	99.046	1.00	42.78
1651	C	THR	A	333	-24.981	25.425	96.865	1.00	34.33
1652	O	THR	A	333	-25.642	26.372	96.398	1.00	33.08
1653	N	TYR	A	334	-24.713	24.319	96.190	1.00	34.09
1654	CA	TYR	A	334	-25.181	24.137	94.830	1.00	33.28
1655	CB	TYR	A	334	-24.748	22.746	94.425	1.00	34.15
1656	CG	TYR	A	334	-25.241	22.198	93.148	1.00	35.67
1657	CD1	TYR	A	334	-24.367	22.102	92.069	1.00	39.34
1658	CE1	TYR	A	334	-24.765	21.536	90.885	1.00	41.47
1659	CZ	TYR	A	334	-26.025	21.028	90.764	1.00	45.44
1660	OH	TYR	A	334	-26.316	20.439	89.536	1.00	53.44
1661	CE2	TYR	A	334	-26.931	21.076	91.822	1.00	41.49
1662	CD2	TYR	A	334	-26.535	21.644	93.021	1.00	39.26
1663	C	TYR	A	334	-26.682	24.162	94.837	1.00	34.00
1664	O	TYR	A	334	-27.330	24.686	93.921	1.00	32.29
1665	N	GLN	A	335	-27.263	23.490	95.830	1.00	33.92
1666	CA	GLN	A	335	-28.698	23.382	95.856	1.00	34.59
1667	CB	GLN	A	335	-29.136	22.355	96.934	1.00	36.44
1668	CG	GLN	A	335	-28.819	20.855	96.503	1.00	37.94
1669	CD	GLN	A	335	-27.495	20.276	97.085	1.00	40.55
1670	OE1	GLN	A	335	-27.461	19.102	97.552	1.00	37.86
1671	NE2	GLN	A	335	-26.437	21.088	97.108	1.00	36.60
1672	C	GLN	A	335	-29.324	24.794	96.037	1.00	34.20
1673	O	GLN	A	335	-30.282	25.140	95.379	1.00	35.30
1674	N	GLU	A	336	-28.791	25.559	96.942	1.00	32.77

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
1675	CA	GLU	A	336	-29.205	26.915	97.201	1.00	34.44
1676	CB	GLU	A	336	-28.385	27.265	98.440	1.00	36.83
1677	CG	GLU	A	336	-28.352	28.650	99.013	1.00	40.38
1678	CD	GLU	A	336	-27.092	28.866	99.875	1.00	50.58
1679	OE1	GLU	A	336	-25.978	28.319	99.620	1.00	58.53
1680	OE2	GLU	A	336	-27.126	29.678	100.790	1.00	40.31
1681	C	GLU	A	336	-28.995	27.811	95.873	1.00	33.80
1682	O	GLU	A	336	-29.877	28.563	95.449	1.00	31.17
1683	N	THR	A	337	-27.868	27.635	95.191	1.00	32.08
1684	CA	THR	A	337	-27.662	28.368	93.945	1.00	31.48
1685	CB	THR	A	337	-26.235	28.047	93.405	1.00	30.08
1686	OG1	THR	A	337	-25.313	28.487	94.390	1.00	33.00
1687	CG2	THR	A	337	-25.906	28.929	92.159	1.00	28.28
1688	C	THR	A	337	-28.724	28.055	92.919	1.00	29.52
1689	O	THR	A	337	-29.235	28.932	92.247	1.00	28.46
1690	N	TYR	A	338	-29.027	26.756	92.754	1.00	30.17
1691	CA	TYR	A	338	-30.049	26.309	91.844	1.00	31.26
1692	CB	TYR	A	338	-30.212	24.805	92.063	1.00	33.22
1693	CG	TYR	A	338	-31.212	24.185	91.144	1.00	39.22
1694	CD1	TYR	A	338	-30.800	23.567	89.964	1.00	43.19
1695	CE1	TYR	A	338	-31.709	22.969	89.124	1.00	48.41
1696	CZ	TYR	A	338	-33.058	23.003	89.460	1.00	51.06
1697	OH	TYR	A	338	-33.992	22.431	88.628	1.00	55.33
1698	CE2	TYR	A	338	-33.479	23.615	90.622	1.00	46.29
1699	CD2	TYR	A	338	-32.560	24.179	91.462	1.00	40.97
1700	C	TYR	A	338	-31.396	27.002	92.147	1.00	30.29
1701	O	TYR	A	338	-32.102	27.472	91.277	1.00	29.01
1702	N	ALA	A	339	-31.739	27.026	93.411	1.00	29.94
1703	CA	ALA	A	339	-32.984	27.737	93.804	1.00	30.96
1704	CB	ALA	A	339	-33.149	27.684	95.338	1.00	30.49
1705	C	ALA	A	339	-32.960	29.196	93.377	1.00	29.24
1706	O	ALA	A	339	-33.915	29.676	92.798	1.00	30.50
1707	N	ARG	A	340	-31.867	29.875	93.686	1.00	28.80
1708	CA	ARG	A	340	-31.708	31.285	93.348	1.00	29.69
1709	CB	ARG	A	340	-30.375	31.804	93.896	1.00	29.56
1710	CG	ARG	A	340	-30.447	31.776	95.494	1.00	34.62
1711	CD	ARG	A	340	-31.154	32.954	96.011	1.00	39.53
1712	NE	ARG	A	340	-30.493	34.042	95.311	1.00	45.06
1713	CZ	ARG	A	340	-29.323	34.499	95.716	1.00	45.59
1714	NH1	ARG	A	340	-28.683	35.456	95.038	1.00	44.01
1715	NH2	ARG	A	340	-28.835	33.995	96.846	1.00	44.77
1716	C	ARG	A	340	-31.871	31.547	91.858	1.00	29.56
1717	O	ARG	A	340	-32.649	32.431	91.413	1.00	29.84
1718	N	ILE	A	341	-31.248	30.679	91.087	1.00	29.70
1719	CA	ILE	A	341	-31.279	30.831	89.641	1.00	27.75
1720	CB	ILE	A	341	-30.265	29.851	89.077	1.00	27.48
1721	CG1	ILE	A	341	-28.835	30.335	89.281	1.00	24.64
1722	CD1	ILE	A	341	-27.801	29.268	88.849	1.00	27.34
1723	CG2	ILE	A	341	-30.531	29.617	87.612	1.00	28.09
1724	C	ILE	A	341	-32.653	30.582	89.129	1.00	28.03
1725	O	ILE	A	341	-33.236	31.391	88.388	1.00	29.33

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
1726	N	SER	A	342	-33.258	29.478	89.585	1.00	30.95
1727	CA	SER	A	342	-34.581	29.093	89.125	1.00	31.90
1728	CB	SER	A	342	-34.973	27.779	89.822	1.00	33.11
1729	OG	SER	A	342	-36.337	27.538	89.665	1.00	42.55
1730	C	SER	A	342	-35.593	30.214	89.400	1.00	32.49
1731	O	SER	A	342	-36.445	30.492	88.565	1.00	35.12
1732	N	ARG	A	343	-35.471	30.872	90.559	1.00	31.84
1733	CA	ARG	A	343	-36.386	31.949	90.917	1.00	32.56
1734	CB	ARG	A	343	-36.532	32.017	92.470	1.00	33.12
1735	CG	ARG	A	343	-37.178	30.751	93.099	1.00	36.80
1736	CD	ARG	A	343	-36.953	30.623	94.628	1.00	43.39
1737	NE	ARG	A	343	-37.670	29.540	95.344	1.00	52.05
1738	CZ	ARG	A	343	-38.085	28.360	94.847	1.00	55.23
1739	NH1	ARG	A	343	-37.862	28.015	93.587	1.00	58.10
1740	NH2	ARG	A	343	-38.717	27.495	95.654	1.00	55.82
1741	C	ARG	A	343	-35.914	33.324	90.386	1.00	32.02
1742	O	ARG	A	343	-36.648	34.286	90.481	1.00	31.13
1743	N	VAL	A	344	-34.717	33.360	89.766	1.00	32.93
1744	CA	VAL	A	344	-34.045	34.613	89.312	1.00	33.02
1745	CB	VAL	A	344	-34.600	35.259	88.032	1.00	33.79
1746	CG1	VAL	A	344	-33.546	36.165	87.403	1.00	33.57
1747	CG2	VAL	A	344	-35.020	34.205	87.041	1.00	34.92
1748	C	VAL	A	344	-33.993	35.587	90.479	1.00	31.91
1749	O	VAL	A	344	-34.392	36.741	90.393	1.00	32.52
1750	N	GLU	A	345	-33.500	35.117	91.597	1.00	33.06
1751	CA	GLU	A	345	-33.507	35.977	92.743	1.00	35.54
1752	CB	GLU	A	345	-34.047	35.248	93.988	1.00	37.02
1753	CG	GLU	A	345	-33.651	33.818	94.122	1.00	44.67
1754	CD	GLU	A	345	-34.183	33.209	95.428	1.00	54.61
1755	OE1	GLU	A	345	-34.610	33.982	96.347	1.00	58.06
1756	OE2	GLU	A	345	-34.139	31.965	95.554	1.00	58.84
1757	C	GLU	A	345	-32.132	36.606	92.961	1.00	33.87
1758	O	GLU	A	345	-31.186	35.950	93.332	1.00	33.72
1759	N	PHE	A	346	-32.045	37.894	92.694	1.00	32.77
1760	CA	PHE	A	346	-30.811	38.628	92.902	1.00	32.91
1761	CB	PHE	A	346	-29.903	38.502	91.657	1.00	33.13
1762	CG	PHE	A	346	-30.431	39.197	90.469	1.00	34.17
1763	CD1	PHE	A	346	-31.338	38.570	89.647	1.00	36.56
1764	CE1	PHE	A	346	-31.838	39.183	88.527	1.00	35.71
1765	CZ	PHE	A	346	-31.465	40.474	88.220	1.00	38.88
1766	CE2	PHE	A	346	-30.569	41.142	89.037	1.00	38.32
1767	CD2	PHE	A	346	-30.018	40.488	90.146	1.00	39.09
1768	C	PHE	A	346	-31.134	40.106	93.174	1.00	33.06
1769	O	PHE	A	346	-32.209	40.598	92.785	1.00	32.92
1770	N	THR	A	347	-30.225	40.796	93.853	1.00	32.73
1771	CA	THR	A	347	-30.385	42.225	94.108	1.00	33.76
1772	CB	THR	A	347	-30.753	42.502	95.597	1.00	33.91
1773	OG1	THR	A	347	-29.776	41.870	96.415	1.00	35.21
1774	CG2	THR	A	347	-32.067	41.798	96.015	1.00	33.87
1775	C	THR	A	347	-29.025	42.839	93.850	1.00	33.74
1776	O	THR	A	347	-27.998	42.142	93.915	1.00	34.60

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
1777	N	PHE	A	348	-29.028	44.146	93.635	1.00	33.51
1778	CA	PHE	A	348	-27.835	44.911	93.268	1.00	33.28
1779	CB	PHE	A	348	-28.204	45.979	92.254	1.00	32.67
1780	CG	PHE	A	348	-28.626	45.454	90.940	1.00	31.24
1781	CD1	PHE	A	348	-29.962	45.538	90.551	1.00	32.35
1782	CE1	PHE	A	348	-30.374	45.068	89.325	1.00	31.74
1783	CZ	PHE	A	348	-29.433	44.491	88.447	1.00	30.42
1784	CE2	PHE	A	348	-28.090	44.411	88.822	1.00	32.15
1785	CD2	PHE	A	348	-27.695	44.892	90.070	1.00	30.97
1786	C	PHE	A	348	-27.337	45.701	94.453	1.00	35.77
1787	O	PHE	A	348	-28.126	46.255	95.209	1.00	35.76
1788	N	PRO	A	349	-26.025	45.772	94.628	1.00	36.99
1789	CA	PRO	A	349	-25.493	46.699	95.626	1.00	37.46
1790	CB	PRO	A	349	-23.963	46.485	95.567	1.00	38.56
1791	CG	PRO	A	349	-23.670	45.526	94.471	1.00	37.30
1792	CD	PRO	A	349	-24.990	45.029	93.906	1.00	37.24
1793	C	PRO	A	349	-25.883	48.098	95.159	1.00	37.57
1794	O	PRO	A	349	-26.153	48.337	93.990	1.00	36.04
1795	N	ASP	A	350	-25.921	49.055	96.076	1.00	39.36
1796	CA	ASP	A	350	-26.257	50.422	95.693	1.00	40.98
1797	CB	ASP	A	350	-26.206	51.348	96.903	1.00	42.59
1798	CG	ASP	A	350	-27.260	51.031	97.914	1.00	47.11
1799	OD1	ASP	A	350	-27.128	51.620	99.016	1.00	53.92
1800	OD2	ASP	A	350	-28.222	50.225	97.689	1.00	50.42
1801	C	ASP	A	350	-25.351	51.058	94.663	1.00	40.13
1802	O	ASP	A	350	-25.814	51.905	93.909	1.00	40.28
1803	N	PHE	A	351	-24.063	50.736	94.649	1.00	39.85
1804	CA	PHE	A	351	-23.202	51.402	93.673	1.00	39.47
1805	CB	PHE	A	351	-21.718	51.213	93.957	1.00	40.21
1806	CG	PHE	A	351	-21.278	49.784	93.967	1.00	41.11
1807	CD1	PHE	A	351	-21.221	49.082	95.162	1.00	39.89
1808	CE1	PHE	A	351	-20.833	47.761	95.192	1.00	40.56
1809	CZ	PHE	A	351	-20.521	47.111	93.978	1.00	42.46
1810	CE2	PHE	A	351	-20.589	47.826	92.772	1.00	39.35
1811	CD2	PHE	A	351	-20.977	49.124	92.767	1.00	41.22
1812	C	PHE	A	351	-23.543	51.116	92.213	1.00	40.90
1813	O	PHE	A	351	-23.177	51.889	91.325	1.00	41.02
1814	N	VAL	A	352	-24.278	50.042	91.927	1.00	39.58
1815	CA	VAL	A	352	-24.604	49.759	90.531	1.00	38.85
1816	CB	VAL	A	352	-25.223	48.351	90.345	1.00	37.90
1817	CG1	VAL	A	352	-25.491	48.084	88.893	1.00	36.19
1818	CG2	VAL	A	352	-24.271	47.308	90.902	1.00	38.04
1819	C	VAL	A	352	-25.531	50.764	89.905	1.00	39.39
1820	O	VAL	A	352	-26.631	50.985	90.420	1.00	38.87
1821	N	THR	A	353	-25.136	51.309	88.742	1.00	40.16
1822	CA	THR	A	353	-25.943	52.332	88.057	1.00	40.56
1823	CB	THR	A	353	-25.127	53.080	86.987	1.00	41.20
1824	OG1	THR	A	353	-24.703	52.160	85.970	1.00	39.47
1825	CG2	THR	A	353	-23.893	53.625	87.588	1.00	39.13
1826	C	THR	A	353	-27.216	51.852	87.400	1.00	41.64
1827	O	THR	A	353	-27.424	50.664	87.152	1.00	41.19

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
1828	N	GLU	A	354	-28.071	52.816	87.102	1.00	41.67
1829	CA	GLU	A	354	-29.321	52.514	86.485	1.00	43.44
1830	CB	GLU	A	354	-30.191	53.770	86.372	1.00	46.05
1831	CG	GLU	A	354	-30.592	54.252	87.751	1.00	54.41
1832	CD	GLU	A	354	-30.894	53.090	88.684	1.00	64.52
1833	OE1	GLU	A	354	-32.014	52.505	88.550	1.00	68.68
1834	OE2	GLU	A	354	-30.038	52.775	89.551	1.00	67.34
1835	C	GLU	A	354	-29.168	51.828	85.156	1.00	41.54
1836	O	GLU	A	354	-29.908	50.900	84.858	1.00	40.38
1837	N	GLY	A	355	-28.226	52.291	84.353	1.00	40.21
1838	CA	GLY	A	355	-28.041	51.714	83.044	1.00	37.79
1839	C	GLY	A	355	-27.598	50.271	83.170	1.00	36.84
1840	O	GLY	A	355	-28.060	49.403	82.423	1.00	37.14
1841	N	ALA	A	356	-26.684	50.016	84.092	1.00	36.29
1842	CA	ALA	A	356	-26.178	48.669	84.268	1.00	36.41
1843	CB	ALA	A	356	-24.998	48.660	85.206	1.00	35.64
1844	C	ALA	A	356	-27.295	47.794	84.782	1.00	35.70
1845	O	ALA	A	356	-27.490	46.695	84.309	1.00	34.90
1846	N	ARG	A	357	-28.072	48.293	85.745	1.00	36.25
1847	CA	ARG	A	357	-29.186	47.504	86.264	1.00	36.61
1848	CB	ARG	A	357	-29.960	48.250	87.339	1.00	36.86
1849	CG	ARG	A	357	-29.169	48.482	88.582	1.00	34.77
1850	CD	ARG	A	357	-29.988	49.289	89.609	1.00	37.61
1851	NE	ARG	A	357	-29.112	49.640	90.708	1.00	36.40
1852	CZ	ARG	A	357	-29.400	49.468	91.975	1.00	35.35
1853	NH1	ARG	A	357	-30.572	48.952	92.320	1.00	39.15
1854	NH2	ARG	A	357	-28.498	49.787	92.890	1.00	33.56
1855	C	ARG	A	357	-30.165	47.167	85.172	1.00	37.12
1856	O	ARG	A	357	-30.718	46.074	85.153	1.00	37.21
1857	N	ASP	A	358	-30.420	48.132	84.297	1.00	37.24
1858	CA	ASP	A	358	-31.353	47.925	83.226	1.00	37.93
1859	CB	ASP	A	358	-31.614	49.202	82.454	1.00	38.87
1860	CG	ASP	A	358	-32.621	48.984	81.324	1.00	42.76
1861	OD1	ASP	A	358	-33.846	49.000	81.602	1.00	46.16
1862	OD2	ASP	A	358	-32.290	48.788	80.126	1.00	45.46
1863	C	ASP	A	358	-30.868	46.836	82.281	1.00	36.98
1864	O	ASP	A	358	-31.656	45.967	81.884	1.00	36.97
1865	N	LEU	A	359	-29.578	46.860	81.942	1.00	35.72
1866	CA	LEU	A	359	-29.042	45.867	81.031	1.00	35.51
1867	CB	LEU	A	359	-27.595	46.168	80.713	1.00	35.38
1868	CG	LEU	A	359	-27.063	45.779	79.327	1.00	39.30
1869	CD1	LEU	A	359	-25.507	45.577	79.301	1.00	37.82
1870	CD2	LEU	A	359	-27.787	44.681	78.634	1.00	35.07
1871	C	LEU	A	359	-29.127	44.477	81.657	1.00	33.71
1872	O	LEU	A	359	-29.575	43.515	81.028	1.00	32.97
1873	N	ILE	A	360	-28.679	44.388	82.900	1.00	32.44
1874	CA	ILE	A	360	-28.646	43.105	83.610	1.00	31.57
1875	CB	ILE	A	360	-27.847	43.253	84.926	1.00	31.85
1876	CG1	ILE	A	360	-26.367	43.490	84.572	1.00	32.47
1877	CD1	ILE	A	360	-25.639	44.299	85.549	1.00	29.24
1878	CG2	ILE	A	360	-27.934	41.956	85.801	1.00	30.72

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
1879	C	ILE	A	360	-30.053	42.521	83.830	1.00	32.40
1880	O	ILE	A	360	-30.265	41.308	83.611	1.00	31.17
1881	N	SER	A	361	-30.996	43.386	84.214	1.00	32.23
1882	CA	SER	A	361	-32.363	42.958	84.445	1.00	34.85
1883	CB	SER	A	361	-33.223	44.060	85.087	1.00	35.23
1884	OG	SER	A	361	-32.814	44.245	86.443	1.00	40.29
1885	C	SER	A	361	-32.969	42.457	83.143	1.00	34.58
1886	O	SER	A	361	-33.734	41.528	83.147	1.00	34.46
1887	N	ARG	A	362	-32.571	43.020	82.017	1.00	35.27
1888	CA	ARG	A	362	-33.116	42.553	80.736	1.00	35.84
1889	CB	ARG	A	362	-32.908	43.595	79.653	1.00	36.24
1890	CG	ARG	A	362	-33.797	44.805	79.768	1.00	42.24
1891	CD	ARG	A	362	-33.312	46.000	78.930	1.00	48.93
1892	NE	ARG	A	362	-34.160	47.177	79.139	1.00	57.80
1893	CZ	ARG	A	362	-34.932	47.717	78.208	1.00	63.64
1894	NH1	ARG	A	362	-34.931	47.208	76.972	1.00	67.52
1895	NH2	ARG	A	362	-35.696	48.771	78.502	1.00	65.50
1896	C	ARG	A	362	-32.525	41.220	80.283	1.00	35.03
1897	O	ARG	A	362	-33.216	40.429	79.634	1.00	36.42
1898	N	LEU	A	363	-31.279	40.939	80.664	1.00	32.41
1899	CA	LEU	A	363	-30.645	39.705	80.279	1.00	32.03
1900	CB	LEU	A	363	-29.133	39.896	80.329	1.00	31.58
1901	CG	LEU	A	363	-28.234	40.365	79.163	1.00	34.89
1902	CD1	LEU	A	363	-28.757	40.467	77.803	1.00	36.09
1903	CD2	LEU	A	363	-27.243	41.450	79.528	1.00	34.69
1904	C	LEU	A	363	-31.027	38.572	81.203	1.00	32.15
1905	O	LEU	A	363	-31.111	37.430	80.776	1.00	33.41
1906	N	LEU	A	364	-31.268	38.857	82.472	1.00	31.16
1907	CA	LEU	A	364	-31.571	37.770	83.428	1.00	32.01
1908	CB	LEU	A	364	-30.963	38.067	84.804	1.00	31.60
1909	CG	LEU	A	364	-29.420	38.146	84.738	1.00	31.16
1910	CD1	LEU	A	364	-28.840	38.468	86.102	1.00	34.77
1911	CD2	LEU	A	364	-28.841	36.783	84.213	1.00	31.53
1912	C	LEU	A	364	-33.088	37.535	83.500	1.00	33.63
1913	O	LEU	A	364	-33.734	37.811	84.487	1.00	33.26
1914	N	LYS	A	365	-33.662	37.065	82.410	1.00	33.41
1915	CA	LYS	A	365	-35.082	36.796	82.393	1.00	35.64
1916	CB	LYS	A	365	-35.718	37.369	81.135	1.00	35.84
1917	CG	LYS	A	365	-35.929	38.880	81.125	1.00	39.34
1918	CD	LYS	A	365	-36.633	39.297	82.400	1.00	46.53
1919	CE	LYS	A	365	-37.698	40.335	82.107	1.00	49.18
1920	NZ	LYS	A	365	-37.064	41.556	81.577	1.00	54.14
1921	C	LYS	A	365	-35.216	35.299	82.375	1.00	35.57
1922	O	LYS	A	365	-34.516	34.626	81.599	1.00	34.77
1923	N	HIS	A	366	-36.084	34.780	83.241	1.00	34.63
1924	CA	HIS	A	366	-36.339	33.372	83.302	1.00	36.28
1925	CB	HIS	A	366	-37.437	33.047	84.346	1.00	35.81
1926	CG	HIS	A	366	-37.567	31.581	84.590	1.00	39.29
1927	ND1	HIS	A	366	-38.186	30.728	83.693	1.00	41.29
1928	CE1	HIS	A	366	-38.111	29.487	84.145	1.00	40.54
1929	NE2	HIS	A	366	-37.446	29.500	85.291	1.00	42.19



### FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1930	CD2	HIS	A	366	-37.088	30.796	85.587	1.00	39.35
1931	C	HIS	A	366	-36.789	32.856	81.911	1.00	37.30
1932	O	HIS	A	366	-36.356	31.798	81.435	1.00	36.00
1933	N	ASN	A	367	-37.684	33.573	81.261	1.00	38.00
1934	CA	ASN	A	367	-38.095	33.069	79.937	1.00	40.10
1935	CB	ASN	A	367	-39.487	33.598	79.658	1.00	40.85
1936	CG	ASN	A	367	-40.080	33.074	78.380	1.00	44.28
1937	OD1	ASN	A	367	-41.276	33.219	78.172	1.00	51.80
1938	ND2	ASN	A	367	-39.271	32.476	77.525	1.00	46.36
1939	C	ASN	A	367	-37.086	33.524	78.875	1.00	39.35
1940	O	ASN	A	367	-36.961	34.709	78.683	1.00	38.80
1941	N	PRO	A	368	-36.397	32.591	78.210	1.00	39.49
1942	CA	PRO	A	368	-35.336	32.903	77.238	1.00	40.08
1943	CB	PRO	A	368	-34.976	31.536	76.624	1.00	39.29
1944	CG	PRO	A	368	-35.451	30.502	77.567	1.00	40.15
1945	CD	PRO	A	368	-36.633	31.136	78.295	1.00	40.09
1946	C	PRO	A	368	-35.824	33.807	76.112	1.00	40.68
1947	O	PRO	A	368	-35.082	34.684	75.656	1.00	38.95
1948	N	SER	A	369	-37.064	33.592	75.664	1.00	42.38
1949	CA	SER	A	369	-37.639	34.437	74.597	1.00	43.99
1950	CB	SER	A	369	-39.033	33.951	74.203	1.00	44.88
1951	OG	SER	A	369	-38.956	32.601	73.740	1.00	48.55
1952	C	SER	A	369	-37.742	35.894	74.995	1.00	44.04
1953	O	SER	A	369	-37.889	36.754	74.140	1.00	44.29
1954	N	GLN	A	370	-37.692	36.186	76.295	1.00	44.21
1955	CA	GLN	A	370	-37.719	37.591	76.721	1.00	45.13
1956	CB	GLN	A	370	-38.437	37.739	78.053	1.00	45.55
1957	CG	GLN	A	370	-39.839	37.121	77.994	1.00	50.14
1958	CD	GLN	A	370	-40.602	37.264	79.300	1.00	56.48
1959	OE1	GLN	A	370	-41.679	36.646	79.474	1.00	60.38
1960	NE2	GLN	A	370	-40.060	38.056	80.230	1.00	55.95
1961	C	GLN	A	370	-36.332	38.231	76.806	1.00	44.45
1962	O	GLN	A	370	-36.210	39.423	77.063	1.00	44.24
1963	N	ARG	A	371	-35.285	37.430	76.631	1.00	43.95
1964	CA	ARG	A	371	-33.915	37.962	76.693	1.00	43.01
1965	CB	ARG	A	371	-32.911	36.827	76.882	1.00	42.30
1966	CG	ARG	A	371	-32.994	36.206	78.279	1.00	36.93
1967	CD	ARG	A	371	-32.118	35.032	78.477	1.00	33.96
1968	NE	ARG	A	371	-32.732	34.134	79.452	1.00	33.75
1969	CZ	ARG	A	371	-32.561	32.828	79.521	1.00	32.13
1970	NH1	ARG	A	371	-33.243	32.141	80.440	1.00	33.40
1971	NH2	ARG	A	371	-31.717	32.197	78.702	1.00	30.58
1972	C	ARG	A	371	-33.641	38.717	75.406	1.00	42.92
1973	O	ARG	A	371	-34.115	38.306	74.374	1.00	43.48
1974	N	PRO	A	372	-32.927	39.831	75.459	1.00	43.09
1975	CA	PRO	A	372	-32.678	40.611	74.234	1.00	42.76
1976	CB	PRO	A	372	-31.890	41.837	74.717	1.00	43.00
1977	CG	PRO	A	372	-31.590	41.648	76.178	1.00	42.62
1978	CD	PRO	A	372	-32.371	40.456	76.678	1.00	43.28
1979	C	PRO	A	372	-31.829	39.874	73.226	1.00	43.31
1980	O	PRO	A	372	-31.191	38.862	73.545	1.00	43.24

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
1981	N	MET	A	373	-31.820	40.378	71.995	1.00	43.19
1982	CA	MET	A	373	-30.928	39.857	70.976	1.00	43.50
1983	CB	MET	A	373	-31.448	40.174	69.585	1.00	44.61
1984	CG	MET	A	373	-32.688	39.421	69.205	1.00	50.78
1985	SD	MET	A	373	-33.173	39.941	67.576	1.00	64.15
1986	CE	MET	A	373	-32.985	41.823	67.726	1.00	59.77
1987	C	MET	A	373	-29.564	40.516	71.172	1.00	42.00
1988	O	MET	A	373	-29.452	41.539	71.841	1.00	39.32
1989	N	LEU	A	374	-28.526	39.926	70.597	1.00	41.82
1990	CA	LEU	A	374	-27.188	40.488	70.727	1.00	43.13
1991	CB	LEU	A	374	-26.194	39.605	70.025	1.00	43.22
1992	CG	LEU	A	374	-25.814	38.411	70.923	1.00	45.40
1993	CD1	LEU	A	374	-24.780	37.453	70.278	1.00	44.95
1994	CD2	LEU	A	374	-25.284	38.861	72.288	1.00	41.96
1995	C	LEU	A	374	-27.192	41.923	70.171	1.00	43.85
1996	O	LEU	A	374	-26.478	42.788	70.667	1.00	43.31
1997	N	ALA	A	375	-27.951	42.152	69.118	1.00	43.58
1998	CA	ALA	A	375	-27.979	43.472	68.494	1.00	44.11
1999	CB	ALA	A	375	-29.028	43.491	67.388	1.00	43.88
2000	C	ALA	A	375	-28.336	44.516	69.517	1.00	43.69
2001	O	ALA	A	375	-27.783	45.616	69.548	1.00	45.16
2002	N	GLU	A	376	-29.265	44.123	70.370	1.00	43.44
2003	CA	GLU	A	376	-29.855	44.996	71.354	1.00	43.12
2004	CB	GLU	A	376	-31.147	44.357	71.836	1.00	43.67
2005	CG	GLU	A	376	-32.103	44.068	70.705	1.00	49.90
2006	CD	GLU	A	376	-33.520	43.811	71.206	1.00	57.55
2007	OE1	GLU	A	376	-33.691	42.679	71.699	1.00	56.12
2008	OE2	GLU	A	376	-34.454	44.705	71.124	1.00	60.58
2009	C	GLU	A	376	-28.969	45.306	72.529	1.00	41.38
2010	O	GLU	A	376	-29.116	46.343	73.152	1.00	42.50
2011	N	VAL	A	377	-28.059	44.394	72.850	1.00	39.33
2012	CA	VAL	A	377	-27.116	44.602	73.948	1.00	37.51
2013	CB	VAL	A	377	-26.405	43.276	74.328	1.00	36.63
2014	CG1	VAL	A	377	-25.281	43.536	75.284	1.00	35.55
2015	CG2	VAL	A	377	-27.416	42.254	74.883	1.00	37.26
2016	C	VAL	A	377	-26.043	45.547	73.449	1.00	37.40
2017	O	VAL	A	377	-25.604	46.436	74.147	1.00	37.91
2018	N	LEU	A	378	-25.621	45.323	72.219	1.00	37.51
2019	CA	LEU	A	378	-24.580	46.115	71.589	1.00	39.81
2020	CB	LEU	A	378	-24.266	45.532	70.217	1.00	40.42
2021	CG	LEU	A	378	-23.393	44.286	70.335	1.00	41.70
2022	CD1	LEU	A	378	-23.067	43.658	68.983	1.00	46.77
2023	CD2	LEU	A	378	-22.130	44.678	71.057	1.00	37.23
2024	C	LEU	A	378	-24.946	47.580	71.442	1.00	41.32
2025	O	LEU	A	378	-24.075	48.445	71.358	1.00	42.45
2026	N	GLU	A	379	-26.244	47.845	71.421	1.00	41.71
2027	CA	GLU	A	379	-26.719	49.178	71.213	1.00	42.63
2028	CB	GLU	A	379	-27.670	49.206	70.018	1.00	44.54
2029	CG	GLU	A	379	-26.995	48.791	68.724	1.00	47.20
2030	CD	GLU	A	379	-27.923	48.707	67.527	1.00	56.88
2031	OE1	GLU	A	379	-29.177	48.664	67.706	1.00	59.40

**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
2032	OE2	GLU	A	379	-27.372	48.665	66.389	1.00	61.82
2033	C	GLU	A	379	-27.401	49.692	72.460	1.00	43.14
2034	O	GLU	A	379	-28.071	50.749	72.435	1.00	43.40
2035	N	HIS	A	380	-27.244	48.966	73.575	1.00	41.24
2036	CA	HIS	A	380	-27.851	49.440	74.793	1.00	40.10
2037	CB	HIS	A	380	-27.681	48.393	75.915	1.00	39.60
2038	CG	HIS	A	380	-28.332	48.789	77.191	1.00	38.52
2039	ND1	HIS	A	380	-29.551	48.279	77.590	1.00	40.40
2040	CE1	HIS	A	380	-29.890	48.824	78.747	1.00	37.68
2041	NE2	HIS	A	380	-28.923	49.643	79.122	1.00	39.48
2042	CD2	HIS	A	380	-27.942	49.644	78.160	1.00	34.37
2043	C	HIS	A	380	-27.163	50.747	75.172	1.00	39.36
2044	O	HIS	A	380	-25.985	50.841	75.006	1.00	39.34
2045	N	PRO	A	381	-27.882	51.732	75.713	1.00	40.21
2046	CA	PRO	A	381	-27.277	53.041	75.975	1.00	40.19
2047	CB	PRO	A	381	-28.439	53.885	76.518	1.00	40.84
2048	CG	PRO	A	381	-29.677	53.167	76.093	1.00	42.96
2049	CD	PRO	A	381	-29.307	51.702	76.106	1.00	40.74
2050	C	PRO	A	381	-26.165	52.971	77.002	1.00	39.71
2051	O	PRO	A	381	-25.239	53.739	76.860	1.00	38.49
2052	N	TRP	A	382	-26.267	52.094	78.015	1.00	37.20
2053	CA	TRP	A	382	-25.213	51.967	79.007	1.00	36.17
2054	CB	TRP	A	382	-25.638	51.046	80.145	1.00	34.80
2055	CG	TRP	A	382	-24.604	50.947	81.203	1.00	35.01
2056	CD1	TRP	A	382	-24.349	51.852	82.170	1.00	36.17
2057	NE1	TRP	A	382	-23.326	51.402	82.975	1.00	39.89
2058	CE2	TRP	A	382	-22.895	50.191	82.505	1.00	36.83
2059	CD2	TRP	A	382	-23.684	49.879	81.391	1.00	34.51
2060	CE3	TRP	A	382	-23.437	48.680	80.716	1.00	37.27
2061	CZ3	TRP	A	382	-22.450	47.843	81.185	1.00	35.85
2062	CH2	TRP	A	382	-21.675	48.196	82.283	1.00	34.82
2063	CZ2	TRP	A	382	-21.887	49.357	82.966	1.00	32.53
2064	C	TRP	A	382	-23.940	51.436	78.346	1.00	36.25
2065	O	TRP	A	382	-22.833	51.887	78.657	1.00	36.89
2066	N	ILE	A	383	-24.090	50.456	77.472	1.00	36.03
2067	CA	ILE	A	383	-22.943	49.924	76.734	1.00	36.79
2068	CB	ILE	A	383	-23.373	48.683	75.892	1.00	36.16
2069	CG1	ILE	A	383	-23.751	47.476	76.802	1.00	34.61
2070	CD1	ILE	A	383	-22.522	46.916	77.531	1.00	34.04
2071	CG2	ILE	A	383	-22.221	48.209	75.038	1.00	35.05
2072	C	ILE	A	383	-22.377	51.014	75.804	1.00	39.31
2073	O	ILE	A	383	-21.172	51.250	75.708	1.00	40.13
2074	N	THR	A	384	-23.268	51.707	75.130	1.00	41.29
2075	CA	THR	A	384	-22.849	52.781	74.221	1.00	44.28
2076	CB	THR	A	384	-24.120	53.418	73.673	1.00	44.01
2077	OG1	THR	A	384	-24.539	52.622	72.568	1.00	48.12
2078	CG2	THR	A	384	-23.822	54.750	73.090	1.00	49.09
2079	C	THR	A	384	-22.006	53.846	74.885	1.00	43.49
2080	O	THR	A	384	-20.980	54.271	74.359	1.00	46.02
2081	N	ALA	A	385	-22.449	54.281	76.044	1.00	42.28
2082	CA	ALA	A	385	-21.779	55.332	76.763	1.00	42.24

### FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2083	CB	ALA	A	385	-22.705	55.884	77.823	1.00	41.95
2084	C	ALA	A	385	-20.509	54.897	77.424	1.00	42.41
2085	O	ALA	A	385	-19.606	55.728	77.660	1.00	43.21
2086	N	ASN	A	386	-20.404	53.612	77.749	1.00	40.11
2087	CA	ASN	A	386	-19.254	53.178	78.478	1.00	38.95
2088	CB	ASN	A	386	-19.696	52.453	79.740	1.00	39.05
2089	CG	ASN	A	386	-20.371	53.392	80.739	1.00	39.22
2090	OD1	ASN	A	386	-19.698	54.080	81.495	1.00	40.98
2091	ND2	ASN	A	386	-21.695	53.396	80.754	1.00	40.56
2092	C	ASN	A	386	-18.195	52.366	77.760	1.00	38.55
2093	O	ASN	A	386	-17.077	52.329	78.212	1.00	37.05
2094	N	SER	A	387	-18.545	51.701	76.682	1.00	39.28
2095	CA	SER	A	387	-17.604	50.833	75.997	1.00	41.73
2096	CB	SER	A	387	-18.322	49.922	75.010	1.00	40.55
2097	OG	SER	A	387	-17.359	49.075	74.356	1.00	42.67
2098	C	SER	A	387	-16.573	51.578	75.172	1.00	43.18
2099	O	SER	A	387	-16.930	52.538	74.482	1.00	43.25
2100	N	SER	A	388	-15.344	51.059	75.181	1.00	44.22
2101	CA	SER	A	388	-14.244	51.555	74.351	1.00	46.24
2102	CB	SER	A	388	-12.908	51.070	74.888	1.00	46.39
2103	OG	SER	A	388	-12.725	51.591	76.195	1.00	49.91
2104	C	SER	A	388	-14.358	51.150	72.894	1.00	46.36
2105	O	SER	A	388	-15.115	50.231	72.549	1.00	48.50
2106	O1A	ADP	X2001		-9.414	25.400	78.378	1.00	28.64
2107	PA	ADP	X2001		-9.486	25.363	79.862	1.00	30.26
2108	O2A	ADP	X2001		-10.590	26.255	80.350	1.00	28.31
2109	O3A	ADP	X2001		-9.587	23.880	80.555	1.00	30.98
2110	PB	ADP	X2001		-10.917	23.134	80.991	1.00	31.28
2111	O3B	ADP	X2001		-11.692	24.139	81.826	1.00	28.29
2112	O2B	ADP	X2001		-10.390	21.986	81.811	1.00	35.80
2113	O1B	ADP	X2001		-11.688	22.740	79.755	1.00	28.57
2114	O5*	ADP	X2001		-8.144	25.872	80.503	1.00	30.75
2115	C5*	ADP	X2001		-8.004	25.866	81.924	1.00	30.70
2116	C4*	ADP	X2001		-7.217	27.124	82.368	1.00	29.95
2117	O4*	ADP	X2001		-5.951	27.178	81.679	1.00	28.79
2118	C1*	ADP	X2001		-5.642	28.545	81.342	1.00	29.10
2119	C2*	ADP	X2001		-6.747	29.415	81.899	1.00	26.58
2120	O2*	ADP	X2001		-6.392	29.725	83.238	1.00	34.16
2121	C3*	ADP	X2001		-7.895	28.436	81.993	1.00	29.24
2122	O3*	ADP	X2001		-8.952	28.763	82.864	1.00	32.70
2123	N9	ADP	X2001		-5.577	28.628	79.892	1.00	29.80
2124	C8	ADP	X2001		-6.337	27.843	79.041	1.00	30.16
2125	N7	ADP	X2001		-6.028	28.206	77.750	1.00	29.74
2126	C5	ADP	X2001		-5.143	29.196	77.814	1.00	26.13
2127	C6	ADP	X2001		-4.519	29.877	76.813	1.00	29.08
2128	N6	ADP	X2001		-4.713	29.555	75.506	1.00	25.43
2129	C4	ADP	X2001		-4.835	29.464	79.141	1.00	28.26
2130	N3	ADP	X2001		-3.975	30.435	79.478	1.00	30.28
2131	C2	ADP	X2001		-3.350	31.144	78.490	1.00	31.73
2132	N1	ADP	X2001		-3.633	30.829	77.180	1.00	29.64
2133	O	HOH	X3001		-9.988	28.798	79.067	1.00	31.10

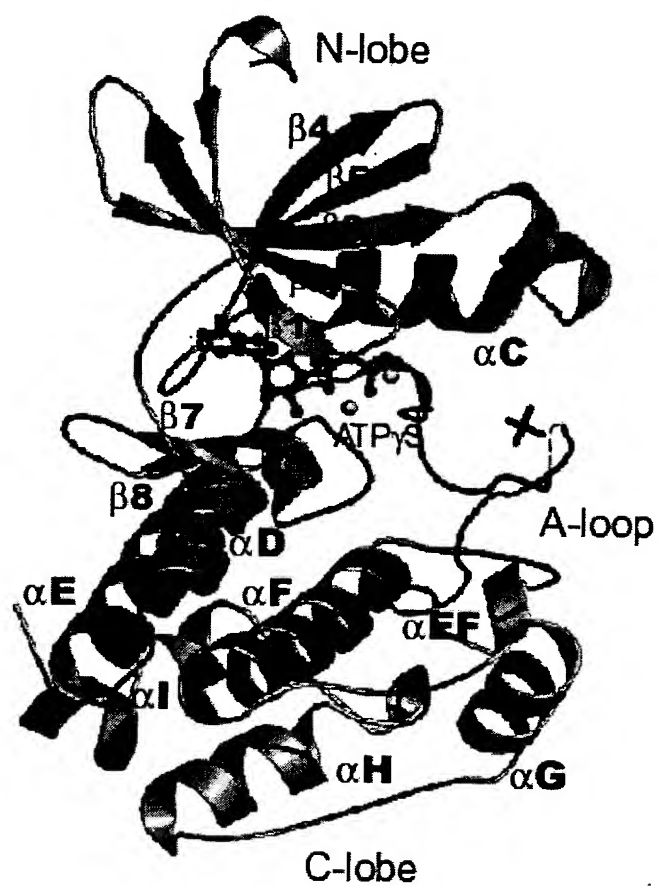
**FIGURE 3 (Cont.)**

A	B	C	D	E	F	G	H	I	J
2134	O	HOH	X3003		-14.393	22.868	80.872	1.00	27.85
2135	O	HOH	X3004		-13.728	20.345	80.020	1.00	45.36
2136	O	HOH	X3005		-26.951	31.694	86.552	1.00	30.10
2137	O	HOH	X3006		-22.935	30.435	78.351	1.00	36.29
2138	O	HOH	X3007		-30.168	16.939	71.846	1.00	45.13
2139	O	HOH	X3008		-18.066	25.328	75.601	1.00	31.20
2140	O	HOH	X3009		-11.548	26.843	82.941	1.00	36.99
2141	O	HOH	X3010		-8.649	27.311	76.774	1.00	31.45
2142	O	HOH	X3011		-37.854	36.557	85.013	1.00	38.02
2143	O	HOH	X3012		-27.723	38.845	94.275	1.00	37.13
2144	O	HOH	X3013		-16.636	24.694	78.361	1.00	32.
2145	O	HOH	X3014		-8.241	35.027	68.248	1.00	33.00
2146	O	HOH	X3015		-0.912	17.916	82.933	1.00	36.14
2147	O	HOH	X3017		-15.066	34.944	89.120	1.00	42.99
2148	O	HOH	X3018		-22.824	25.783	92.176	1.00	46.76
2149	O	HOH	X3021		-11.944	23.669	84.418	1.00	39.47
2150	O	HOH	X3022		-12.703	21.499	77.561	1.00	40.61
2151	O	HOH	X3023		-37.367	42.995	79.960	1.00	59.45
2152	O	HOH	X3024		-5.576	15.379	86.195	1.00	66.48
2153	O	HOH	X3026		-8.353	43.652	79.479	1.00	44.84
2154	O	HOH	X3027		-23.236	19.714	67.938	1.00	47.17
2155	O	HOH	X3028		-10.809	32.568	66.377	1.00	35.26
2156	O	HOH	X3029		-15.673	31.938	88.442	1.00	44.34
2157	O	HOH	X3030		-0.223	35.059	71.257	1.00	55.88
2158	O	HOH	X3031		-20.254	50.297	89.242	1.00	49.49
2159	O	HOH	X3032		-4.408	26.185	61.520	1.00	57.94
2160	O	HOH	X3033		-6.464	20.470	80.244	1.00	42.32
2161	O	HOH	X3034		-26.908	54.727	81.094	1.00	46.09
2162	O	HOH	X3036		-3.500	31.862	81.803	1.00	43.64
2163	O	HOH	X3037		-28.118	35.557	69.369	1.00	53.58
2164	O	HOH	X3038		-26.182	36.321	65.264	1.00	49.67
2165	O	HOH	X3039		14.155	34.581	65.299	1.00	48.35
2166	O	HOH	X3040		-34.861	43.555	76.702	1.00	53.19
2167	O	HOH	X3041		-39.173	35.975	82.307	1.00	45.97
2168	O	HOH	X3043		-14.153	39.758	92.741	1.00	38.14
2169	O	HOH	X3044		-17.759	51.104	95.196	1.00	63.77
2170	O	HOH	X3045		-17.674	46.814	68.492	1.00	55.41
2171	O	HOH	X3046		-21.016	27.883	83.182	1.00	40.34
2172	O	HOH	X3047		-32.376	28.743	75.835	1.00	35.07
2173	O	HOH	X3048		-26.582	54.610	84.614	1.00	51.10
2174	O	HOH	X3049		-28.989	37.779	69.028	1.00	45.59
2175	O	HOH	X3050		1.044	35.132	80.541	1.00	40.83
2176	O	HOH	X3051		-18.143	48.279	89.631	1.00	35.13
2177	O	HOH	X3052		-22.772	50.169	87.633	1.00	35.90
2178	O	HOH	X3054		-28.242	40.105	67.233	1.00	39.46
2179	O	HOH	X3055		-5.648	27.887	86.644	1.00	45.28
2180	O	HOH	X3056		-22.278	29.579	81.107	1.00	46.99
2181	O	HOH	X3057		-21.804	27.943	85.859	1.00	31.17
2182	O	HOH	X3058		-19.327	55.542	84.158	1.00	69.06
2183	O	HOH	X3059		-16.658	53.812	86.138	1.00	76.39
2184	O	HOH	X3060		-11.616	48.407	86.048	1.00	44.96

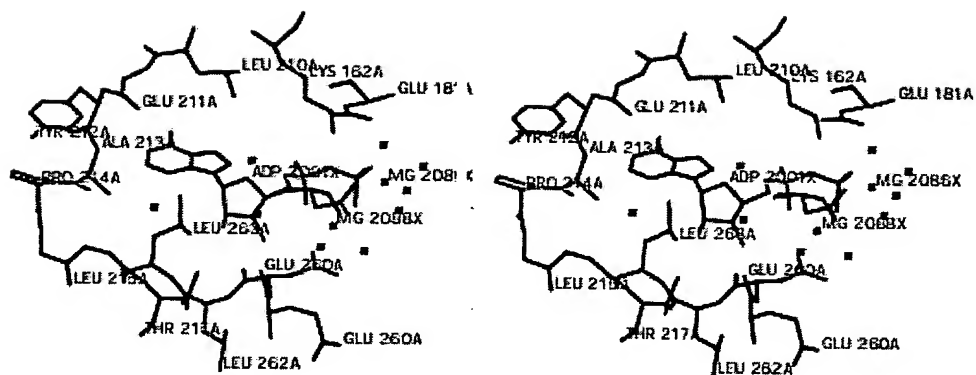
### FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2185	O	HOH	X3061		-35.280	41.364	78.456	1.00	43.63
2186	O	HOH	X3062		-35.848	29.209	81.326	1.00	50.09
2187	O	HOH	X3063		-20.386	19.911	74.001	1.00	46.93
2188	O	HOH	X3064		-5.444	37.823	84.054	1.00	35.84
2189	O	HOH	X3066		-2.738	38.173	71.721	1.00	47.11
2190	O	HOH	X3067		-3.973	35.760	72.248	1.00	33.90
2191	O	HOH	X3068		-29.746	39.136	96.635	1.00	62.80
2192	O	HOH	X3070		-14.064	25.472	82.227	1.00	31.69
2193	O	HOH	X2089		-4.484	33.261	84.056	1.00	47.20
2194	O	HOH	X2090		-9.895	27.055	74.329	1.00	27.24
2195	O	HOH	X2091		-0.170	31.678	70.061	1.00	29.25
2196	O	HOH	X2092		-1.106	31.853	83.735	1.00	53.32
2197	O	HOH	X2093		-25.264	41.053	66.798	1.00	59.10
2198	O	HOH	X2094		-25.466	43.888	65.479	1.00	69.73
2199	O	HOH	X2095		-32.272	31.292	69.214	1.00	67.50
2200	O	HOH	X2096		-24.385	33.367	89.916	1.00	31.89
2201	O	HOH	X2097		-14.677	21.587	82.263	1.00	41.33
2202	O	HOH	X2098		-15.335	22.257	78.530	1.00	36.43
2203	O	HOH	X2099		-11.146	29.804	67.165	1.00	47.94
2204	O	HOH	X2100		-9.610	28.214	65.560	1.00	46.43
2205	MG	MG	X2086		-13.528	22.597	79.198	1.00	12.09
2206	MG	MG	X2088		-12.337	25.921	81.074	1.00	12.20
2207	P	PO4	X2002		-24.838	17.852	76.312	1.00	54.63
2208	O1	PO4	X2002		-24.694	18.499	74.963	1.00	59.50
2209	O2	PO4	X2002		-26.204	17.207	76.361	1.00	64.72
2210	O3	PO4	X2002		-23.779	16.793	76.532	1.00	57.00
2211	O4	PO4	X2002		-24.798	18.859	77.420	1.00	60.01

**FIGURE 4**



**FIGURE 5**





# FIGURE 6

